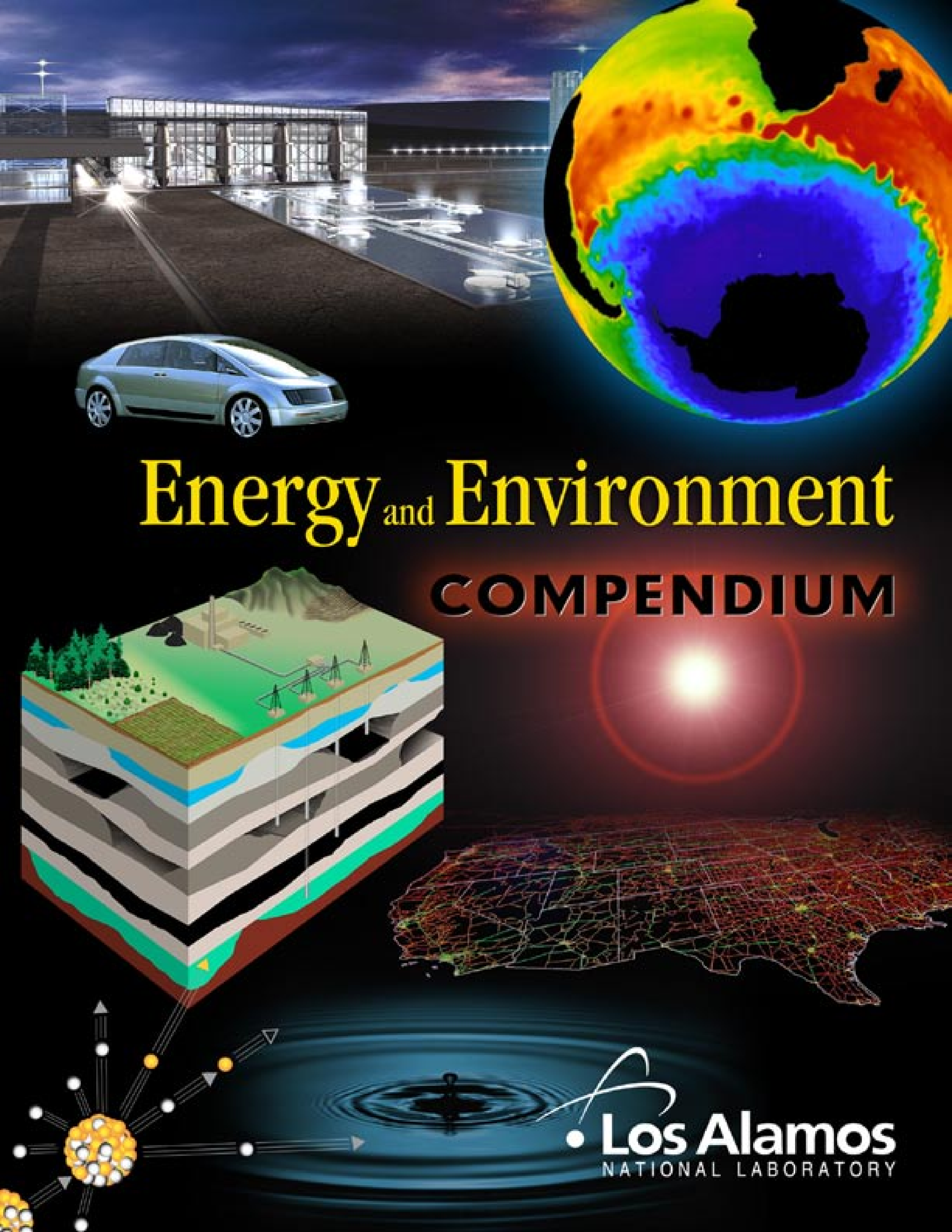
Energy and Environment

COMPENDIUM



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A Comprehensive Approach to National Security

While the nation is preoccupied with hostile threats from abroad, it is easy to forget that other issues could undermine our national security and well-being. Chief among these are the intertwined issues of energy production and environmental sustainability. The nation's security and economic stability rely on sufficient energy supplies and environmentally sound practices of energy production and use. Yet parts of the U.S. have already experienced shortages as electricity demand increases far more rapidly than new generating capacity, and 52% of the nation's primary transportation fuel source is imported from an unstable foreign market (projections show those imports at 70% by 2020). U.S. dependence on these oil-rich regions has had, and continues to have, a direct impact on national security.

Furthermore, increases in atmospheric carbon, caused by current methods of energy production and use, threaten to change the climate in potentially disastrous ways that are little understood at present. The burning of fossil fuels has raised atmospheric levels of carbon dioxide to 380 ppm, significantly higher than at any other time within the last 420,000 years. The effects of this greenhouse gas may become intolerable as those levels approach 500 ppm by the middle of the century. As we reach and exceed this limit, polar ice caps will melt, ocean salinity will decrease, ocean currents may reverse, and life on Earth could change irreversibly.

The nation's, and the world's, greatest challenge over the next several decades will be to halt the progress of global warming but still provide enough energy to maintain a high quality of life in developed countries while raising the standard of living in developing regions of the world. To meet this challenge we must

- transition to energy sources that do not produce greenhouse gases,
- capture and store CO_2 from continued fossil fuel use during the transition period,
- reduce fuel consumption through increased efficiency, and
- protect diminishing water resources by developing less water-intensive energy generation methods.

Los Alamos National Laboratory, a science and technology pioneer and leader in defending America for over 50 years, recognizes that U.S. national security now extends far beyond the need for a strong military defense. Because so much of national stability in the 21st century revolves around issues of energy and the environment, Los Alamos's integrated Energy and Environment Program is applying the Laboratory's multidisciplinary expertise, which has served the nation so well in nuclear defense, to solve national issues of energy security and the interrelated global issues of environmental sustainability. The Laboratory is leading initiatives to

- ensure a stable, non-polluting supply of energy for the future;
- modernize and increase the efficiency of the nation's energy infrastructure;
- prevent carbon emissions from entering or remaining in the atmosphere;
- increase the safety and viability of nuclear energy production;
- ensure an abundant and clean supply of water;

Los Alamos National Laboratory in northern New Mexico.

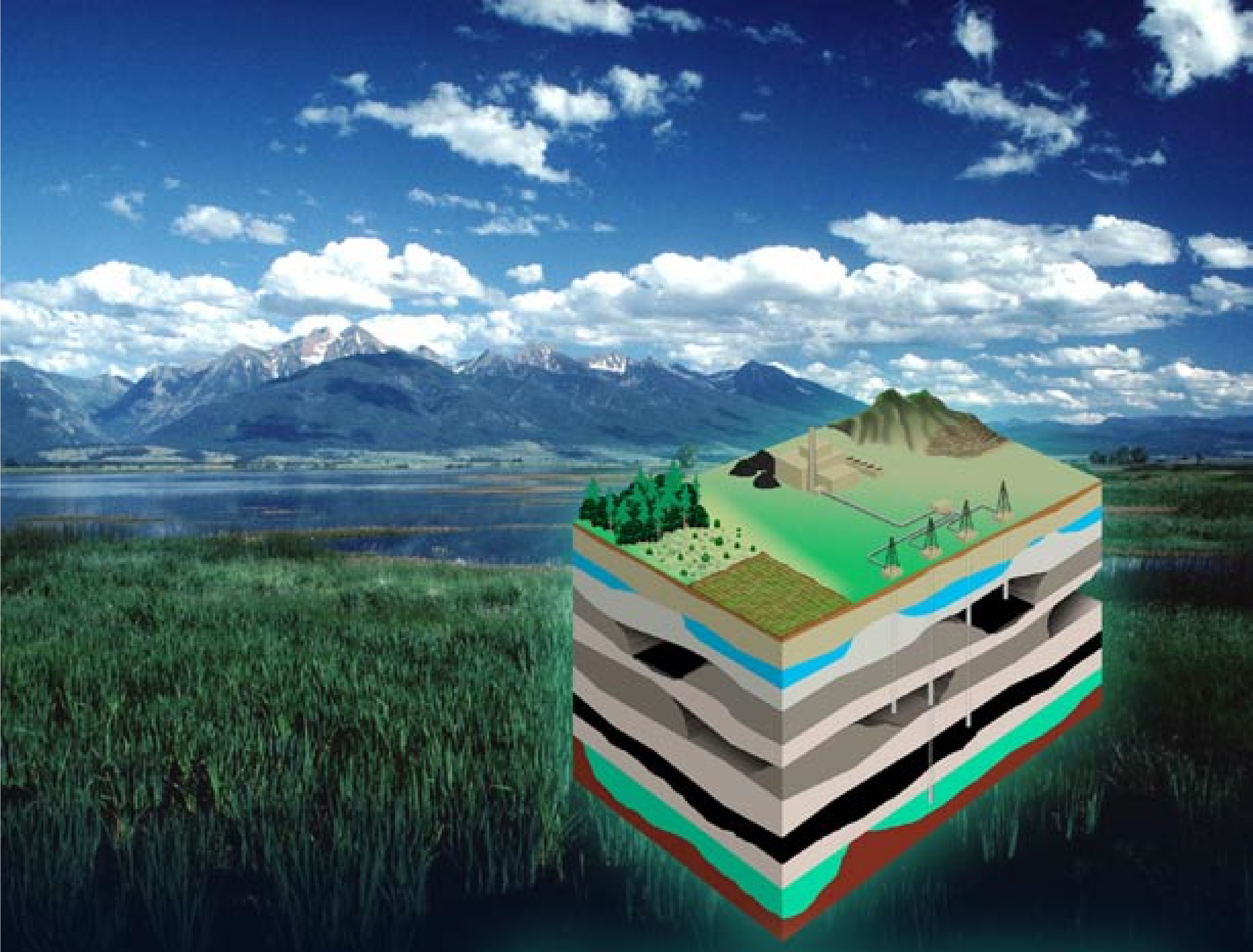
- simulate and understand the interdependencies of infrastructure systems; and
- model and predict the effects of climate change.

The nation's huge investment in Los Alamos National Laboratory has fostered a host of unique scientific and technological capabilities that can be applied to many challenges apart from military defense. Recognizing this, many of Los Alamos's scientists and engineers have asked, what if we could take the Laboratory's capabilities and

- convert the U.S. transportation economy into a clean, domestically-fueled hydrogen-based system?
- continue to use coal, our cheapest and most abundant resource, but eliminate the harmful greenhouse gas emissions?
- replace our electricity transmission lines with superconducting cables that transfer *all* the electricity from generators to users with no current loss?
- prevent global climate change by accelerating natural carbon intake processes (biological and mineral)?
- store industrial CO_2 emissions in safe geological wells and at the same time use them to increase production of natural gas?
- reduce the hazards of generating nuclear energy by making the waste less harmful and unsuitable for weapons production?
- predict the regional effects of global climate change and address problems before they arise?
- predict any harmful effects of electricity deregulation before they occur, or foresee vulnerabilities in our electric and transportation systems before they fail or are exploited maliciously?
- make untapped, non-potable water reserves available for industrial use and electricity generation to relieve overburdened freshwater resources?

Los Alamos already has a long history of turning these and other related visions into reality, and the Laboratory has long worked with industry to bring innovations into practical development and use.

This publication presents much of the research and development that Los Alamos National Laboratory is performing to ensure our nation's energy security and environmental sustainability. To obtain the most current information about Los Alamos National Laboratory's energy and environment research and development, visit us on the Internet at **http://www.lanl.gov/energy**.



CARBON

Energy and Environment Compendium

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Carbon Fuel Cycle Research at Los Alamos National Laboratory

Carbon Fuel Cycle Research at Los Alamos National Laboratory

Fossil fuels represent an abundant and cheap domestic resource for energy, yet increasing levels of atmospheric carbon dioxide (CO_2, which is by volume the largest by-product of fossil-fuel combustion) are challenging their continued use.

Early in 2002, the President announced the need for a "new environmental approach" to the use of fossil fuels, recognizing the challenge of reducing the intensity of greenhouse gas emissions (particularly carbon dioxide) while sustaining economic growth. To meet this challenge, Los Alamos National Laboratory is leveraging a range of theoretical and experimental capabilities to identify new approaches to improving the efficiency of the carbon fuel cycle and minimizing its environmental impact.

The Los Alamos effort is focused on integration of all components of the carbon fuel cycle, including

- Extraction of fossil fuels (oil, gas, coal, hydrates) from the earth;
- Utilization of fossil fuels to produce electricity or to produce a carbon-free energy carrier (e.g., hydrogen);
- Distribution of the electricity/energy carrier to the end user;
- Separation of mixed gases (e.g., from synthesis gases or flue gases);
- Transportation of gas via pipelines; and
- Storage of produced carbon dioxide in a safe and environmentally sound manner.

In addition to the anthropogenic carbon fuel cycle, natural carbon cycles actively move carbon between various earth compartments, such as between the atmosphere and ocean or between terrestrial systems and the atmosphere. These cycles can provide important insights into possible engineered approaches. Moreover, any engineered solution must factor in the coupling between anthropogenic and natural carbon cycles. Los Alamos efforts are focused on understanding both anthropogenic and natural carbon cycles as well as their coupling. For example, the Los Alamos Parallel Ocean Program is being used to understand the impact that biogeochemical carbon cycling in the ocean has on ocean-atmosphere dynamics.

Current Scientific Challenges in Carbon Fuel Cycle Research

To effectively manage the carbon fuel cycle, we must overcome significant technical and scientific challenges, including

- Storing large volumes of carbon dioxide safely and permanently with minimal environmental impact;
- Separating carbon dioxide from mixed-gas streams;
- Improving the efficiency of energy production/conversion;
- Elucidating the complex interplay between carbon cycles and climate; and
- Expanding U.S. fossil fuel reserves.

Los Alamos's Capability Areas in Carbon Fuel Cycle Research

To support its core-mission activities, Los Alamos has developed a suite of unique capabilities that are now being applied to carbon fuel cycle issues. These capabilities fall into several broad categories:

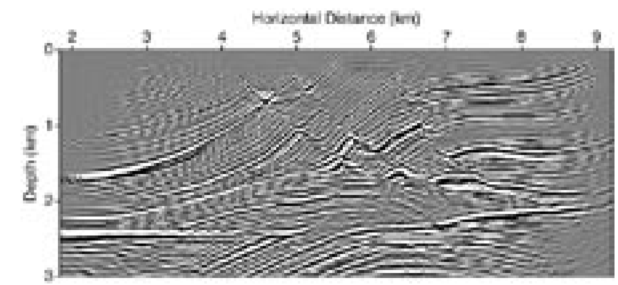
- Monitoring and measurement,
- Catalysis,
- Theory,
- Advanced concepts,
- Separations, and
- Science-based prediction for engineered geological systems.

Seismic and Acoustic Methods to Improve Subsurface Imaging

The Challenge: Imaging Complex Subsurface Structures

The petroleum industry's primary technique to determine where to drill for oil and gas exploration is seismic imaging. Today, new oil and gas exploration targets are in geologies that are increasingly difficult to characterize, and drilling costs are rising. With current methods and technologies, less than 2% of the 7,000 trillion cubic feet of natural gas in the Rocky Mountains' low permeability or "tight" reservoirs can be economically produced. Innovations in acoustic and seismic imaging technologies and methods are vital to future oil and gas extraction.

Los Alamos Innovation: Novel Application of Theory and Interpretation



Los Alamos has developed expertise in characterizing structures in the Earth's subsurface, including (1) seismic modeling and imaging, and (2) monitoring and interpreting seismicity induced by fluid injections. Los Alamos and its partners have produced several breakthroughs:

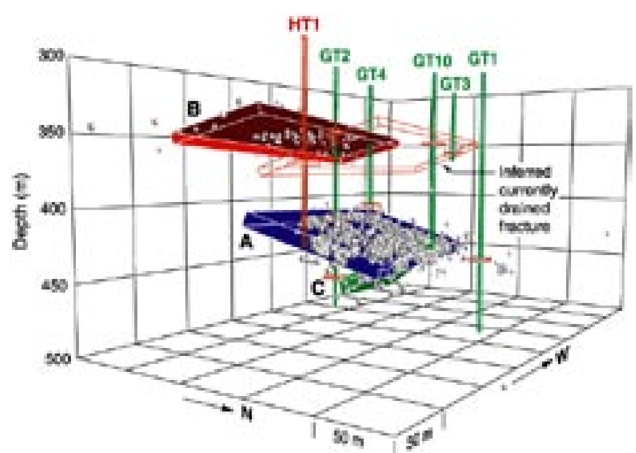
- Seismic imaging based on wave equations;
- Patented methods for imaging and characterizing materials using nonlinear effects in wave propagation;
- Numerical datasets for testing imaging and characterization methods;
- Application of time-reversed acoustics to characterize elastic materials;
- New methods for measuring and analyzing seismic events induced by changes in volume and fluid pressure;
- More realistic models for petroleum-reservoir geology.

Innovative approaches to theory (wave-equation migration shown above) and practice (high-precision arrival time shown below) can lead to dramatic improvements in seismic imaging.

In the future, Los Alamos researchers may be able to yield further breakthroughs in (1) imaging and characterization; (2) understanding and mapping flow paths for fluids in reservoirs (including the effects of induced seismicity); and (3) improved information from images.

The Impact: Increasing Oil and Gas Production

These Los Alamos projects can enhance productivity from oil and gas reservoirs by (1) reducing the risk of drilling dry wells; (2) extracting more oil and gas from permeable rock; and (3) increasing production from existing oil and gas fields. By investigating, testing, validating success, and transferring new technology to the petroleum industry, Los Alamos can help open up substantial new oil and gas resources.



Seismic Stimulation to Recover More Oil and Gas

The Challenge: Maximizing Oil and Gas Extraction

At the average U.S. oil and gas site, about 60% of the oil and gas remains in the ground after primary production. There are compelling reasons to break through current limits to affordable and effective Enhanced Oil Recovery (EOR) methods and technologies, which now rely heavily on water and CO_2 flooding. Seismic stimulation has the potential to meet this need, but is currently unreliable. Results have varied from field to field, and scientists cannot yet predict where it will work and where it will not. The mechanisms involved in seismic stimulation must be far better understood.

Los Alamos Innovation: Seismically Stimulating Fluid Flow

Work on seismic stimulation began with an innovative concept—that low-amplitude, low-frequency (1–500 Hz) seismic stress waves can cause large changes in porous fluid flow in the Earth. Prior to 1992, field tests in the Soviet Union indicated that seismic stimulation could increase oil production rates by 50% or more.

Los Alamos became the first major U.S. research laboratory to investigate seismic stimulation. Los Alamos designed and built a laboratory facility that allows dynamic stress effects on multi-phase fluid flow to be quantified during bench-top experiments on porous core samples. The capabilities of this facility are believed to be unique in the world.

Via experiments performed at its Core Stimulation Facility, Los Alamos is beginning to identify possible guidelines for where and how to apply seismic stimulation effectively. These include (1) using sources that couple energy directly to the core fluids (rather than the solid matrix of the formation) and (2) choosing to stimulate significantly oil-wet (rather than water-wet) reservoirs. Future experiments with field core samples will further quantify these guidelines and help establish additional guidelines.

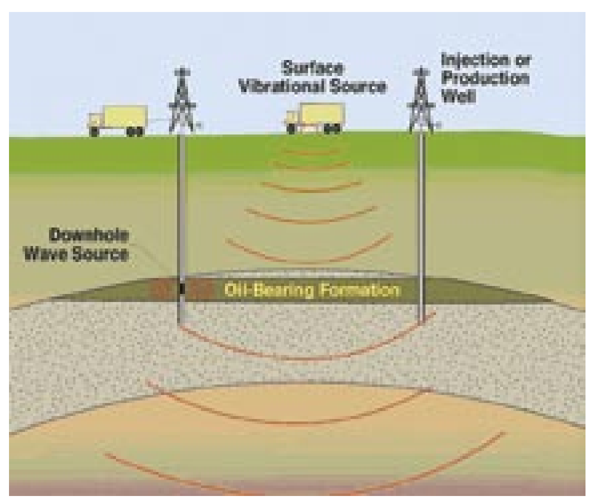
Los Alamos has also initiated industry field tests for developing seismic stimulation sources, and has established numerous collaborations with the oil and gas industry, universities, and other national laboratories. These efforts have increased the credibility of the technology and international scientific interest in the subject.

Early experiments show that stress stimulation can enhance the extraction of Dense Non-Aqueous-Phase Liquid (DNAPL) contaminants from groundwater aquifers. Scientists have also recently identified possible mechanisms coupling stress waves to porous flow.

The Impact: Recovering More Oil and Gas

More research and testing could convert seismic stimulation into an application technology. If so, this capability may (1) allow a greater share of the 60% of oil and gas not recovered at U.S. sites to be recovered and produced; (2) reduce U.S. reliance on foreign oil sources; (3) prevent or delay potential future energy crises; and (4) extend the life of the world's oil and gas supply.

Seismic stimulation can be used to drive fluids in the subsurface.



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Fuel Decarbonization and Catalysis to Reduce Fossil-Fuel Emissions

The Challenge: Reducing Emissions from Fossil Fuel Use

It is well known that producing energy by burning fossil fuels produces carbon dioxide (CO_2), which is widely regarded as a leading greenhouse gas. Government decision-makers struggle with how to reduce emissions of carbon dioxide, particularly in the transportation sector, without putting economic vitality at risk. Solutions are needed to lower the amount of CO_2 produced per unit of energy.

Los Alamos Innovation: More Efficient Catalysis Processes

Advances in energy production technologies could yield such solutions. Since 1995, Los Alamos has brought its expertise, capabilities, and multidisciplinary technical approaches to bear in its carbon-focused Fuel Decarbonization and Catalysis project. First with internal funding and then with funding from the Department of Energy (Office of Science and Office of Energy Efficiency and Renewable Energy) and various chemical and energy industry partners, Los Alamos has investigated carbon catalysis. With both heterogeneous and homogeneous efforts, Los Alamos scientists have built on advantages unique to Los Alamos to achieve the following advances:

- Selectively oxidizing alkanes in heterogeneous catalysis;
- Converting methane to methanol in homogeneous catalysis;
- Using lean nitrogen oxide (NOx) reduction catalysis to enable more fuel-efficient, "lean-burn" engine technologies.

In the future, Los Alamos's efforts can open up a broad range of applications in energy conversion and utilization, including (1) easier conversion and transportation of stranded natural carbon, (2) more affordable carbon conversion and transportation, (3) portable units converting stranded natural gas to a liquid suitable for fuel cell and vehicle use, and (4) further advances in carbon-reduction technology at Los Alamos and elsewhere.

Rapid throughput energy containment reactor boosts catalyst discovery and testing rates.

The Impact: Cleaner, More Efficient Energy

Los Alamos's efforts in this field can (1) increase the efficiency of energy production, (2) reduce fuel consumption in the transportation sector, and (3) reduce greenhouse gas and other emissions.

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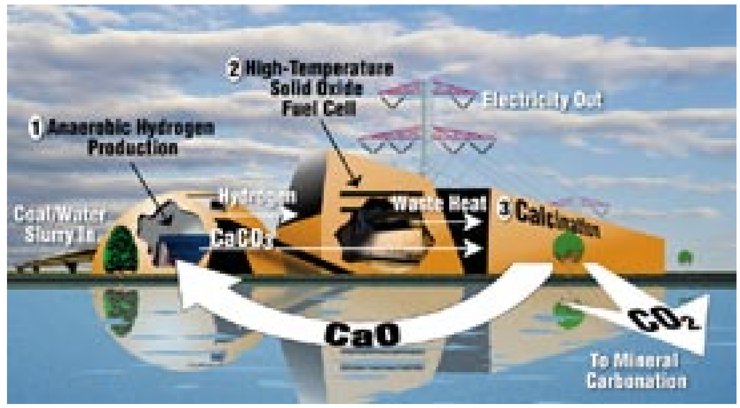
Integrated CO_2 Capture and Energy Conversion to Reduce Coal and Other Fossil-Fuel Emissions

The Challenge: Reducing Emissions in the Energy Sector

Coal is by far the most abundant fossil fuel for the U.S. and the world. However, current methods for using coal to generate energy produce CO_2 and other by-products, creating a variety of environmental challenges. Current approaches to these challenges have evolved largely from modifications to existing technologies and practices. Conventional approaches to purification of CO_2 and its capture focus on upstream separation of oxygen.



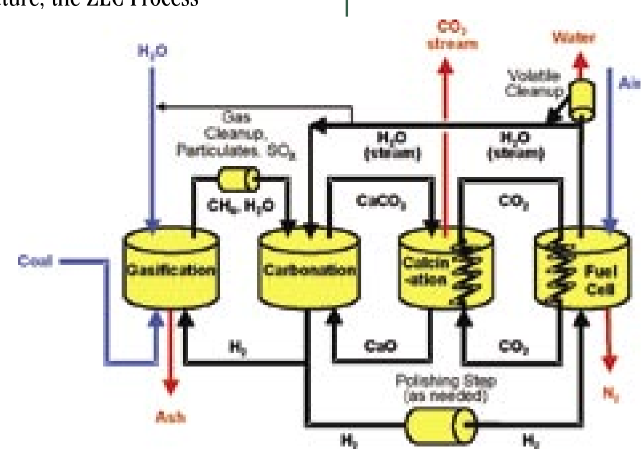
Integration of CO_2 capture with energy conversion could lead to new highly efficient methods for production of hydrogen and electricity from coal. For example, the Zero Emission Coal Process uses lime to shuttle waste heat from high-temperature fuel cells to the shift reaction while separating CO_2 from the gas stream.

Los Alamos Innovation: Integrated CO_2 Separation and Energy Conversion

New environmental challenges provide a driver for considering novel approaches to efficient energy production via coal and other fossil fuels. As part of its portfolio in technologies related to zero-emissions energy production from fossil fuels, Los Alamos has developed a process to improve the efficiency of power production by explicitly integrating the separation and capture of CO_2. This process—often referred to as the ZEC (Zero-Emission Coal) Process—reuses waste heat and includes a lime-CO_2 separation step. Los Alamos's ZEC Process has very high theoretical efficiencies (averaging 70% in one independent evaluation) in purifying CO_2.

Before the ZEC Process is ready for implementation on the pilot scale, critical technical obstacles must be overcome, including (1) development of high-temperature fuel cells that operate at 900˚C and higher and (2) integration of the process elements into a seamless operation. Los Alamos has begun researching these obstacles using internal funding and is currently seeking partners and funding to expand this research and development.

Applications derived from Los Alamos's work on the ZEC Process also include (1) coal-compatible fuel cells, (2) novel trace-element clean-up cycles, and (3) CO_2 mineralization. In the future, the ZEC Process can be combined with a variety of CO_2 storage options. With modifications to various clean-up steps, the ZEC Process can be applied not only to coal but to any fossil fuel or carbon-containing fuel.



The Impact: Abundant, Clean, and Low-Cost Energy

Using the ZEC Process with biomass and a sequestration process, excess CO_2 could actually be removed from the atmosphere. The ZEC Process appears highly promising, and may lead to energy production with zero airborne emissions. If so, the ZEC Process may help secure a sufficient supply of clean, low-cost energy for the U.S. and the world.

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Thermally Optimized Membranes to Separate Gases at High Temperatures

The Challenge: Separating Carbon Dioxide from Mixed Gas

Separating carbon dioxide from mixed-gas streams is the first step in carbon sequestration. To be viable, the separation method must apply to relevant gas streams (including flue gases and synthesis gases) and be able to handle large volumes. The effectiveness of current technologies for separating CO_2 is limited. Amine-based technologies work only at low temperatures. Pressure-swing absorption and cryogenic distillation have significant energy penalties (up to 35%).

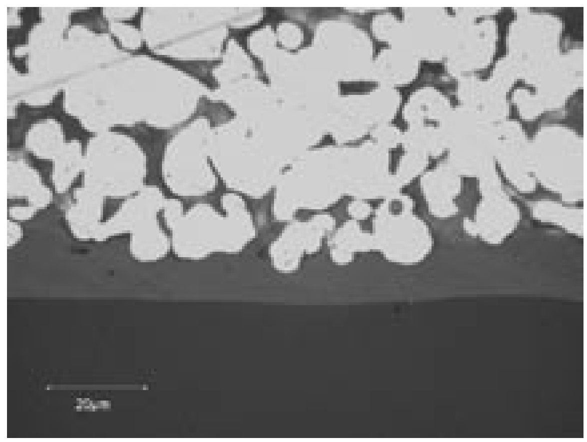
Los Alamos Innovation: A Polymeric-Metallic Composite Membrane

Los Alamos, along with partners, is developing polymeric-metallic composite membranes. These membranes function at significantly higher temperatures (>400˚C) than commercially available polymeric membranes (<150˚C).

To develop and test this membrane system, Los Alamos has exploited its capabilities in materials synthesis, materials characterization, fabrication techniques, and high-temperature membrane testing. To date, Los Alamos and its partners have produced

- The first polymeric-metallic membrane that is selective from room temperature to 400˚C;
- The first polybenzamidizole silicate molecular composites;
- A unique approach to optimizing long-term membrane performance under challenging operating conditions;
- The first-ever simultaneous measurements of gas permeation and membrane compaction at elevated temperatures.

In the future, this project will provide a membrane technology that can be used in a variety of gas separation applications.



Scanning electron microscope image of a polymer-metal composite membrane. Bright spots are metal and the lighter gray is polymer.

The Impact: Less Energy Use in Separating Gases

Polymeric-metallic composite membrane separation is promising. Applications of this technology will reduce energy penalties during the separation process.

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Acoustic Phase Separator to Separate CO_2 from Mixed Gases

The Challenge: Separating CO_2 from Mixed Gases

Carbon sequestration requires separation of CO_2 from mixed-gas streams. Current methods and technologies for separating CO_2 have considerable disadvantages, including (1) high energy penalties (up to 35%), (2) degradation in high-temperature gas streams, and (3) high levels of operative maintenance.

Los Alamos Innovation: The Acoustic Phase Separator

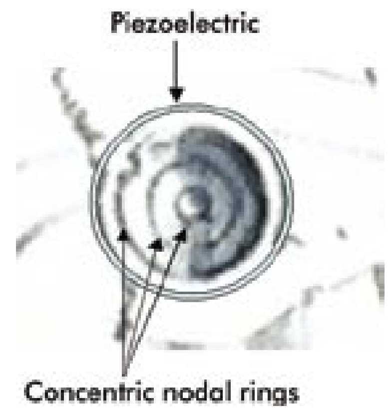
Gases with different properties can be separated using acoustic methods. An acoustic phase separator takes advantage of the sound pressure gradient in a standing wave field in a cylindrical resonance chamber. Los Alamos has patented this novel method, with a second patent pending.

The U.S. Department of Defense has used an acoustic particle concentrator to enhance existing particle counters. The petroleum industry has used acoustic methods and technologies to separate multi-phase liquids.

Los Alamos's acoustic phase separator offers safe, rugged, and ambient operation. The separator is all solid-state with no moving parts, requires no maintenance, and is highly energy-efficient. The temperature of the gas has no effect on operational efficiency. The system is scalable, and multiple units can be stacked together to provide higher throughput. The entire system can be made extremely compact. The separator can be used to separate not only CO_2 but a variety of gases. It can also be used to agglomerate suspended particles in gases and separate those from the gas stream.

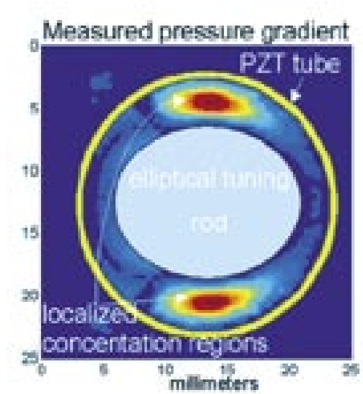
The Impact: Safe and Efficient Separation of Gases

The acoustic phase separator offers a safe, energy-efficient, and cost-effective way to separate mixed gases at high temperatures. The separator uses no cryogen or other chemicals, and it will reduce the cost of the separation process significantly.



Above: Particulate matter in air concentrates at the circular nodal regions of an acoustic standing wave set up inside a piezoelectric hollow cylinder through which the air is flowing.

Below: By breaking the circular symmetry of the cylindrical cavity of the piezoelectric cylinder using an elliptical cross-section insert, the concentration regions can be localized into two spots instead of rings.

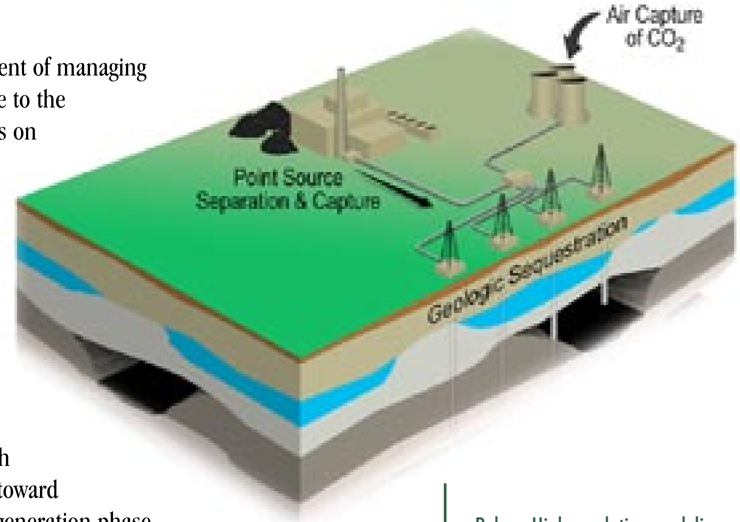


Total Management of CO_2 Through Air Extraction

Air extraction of CO_2 prior to sequestration could complement direct capture from large point sources.

The Challenge: Managing Carbon from All Sources

The control of atmospheric CO_2 levels will likely be an essential component of managing environmental risks associated with the sustained use of fossil fuels. Due to the difficulties of collecting CO_2, current strategies to control emissions focus on capture from large point emitters such as power plants. This strategy neglects past emissions and current emissions from small sources such as automobiles.



Los Alamos Innovation: Directly Extracting CO_2 from the Air

Los Alamos recently proposed the unique concept of directly extracting CO_2 from the atmosphere. This approach focuses on reducing actual atmospheric CO_2 levels rather than reducing just future emissions, which is the idea behind most CO_2 mitigation approaches (including the drive toward renewable sources like wind and solar power). By separating the power generation phase from the CO_2 capture phase, carbon from all sources can be managed without the need for immediate and costly renovations of the infrastructure. Los Alamos's efforts include

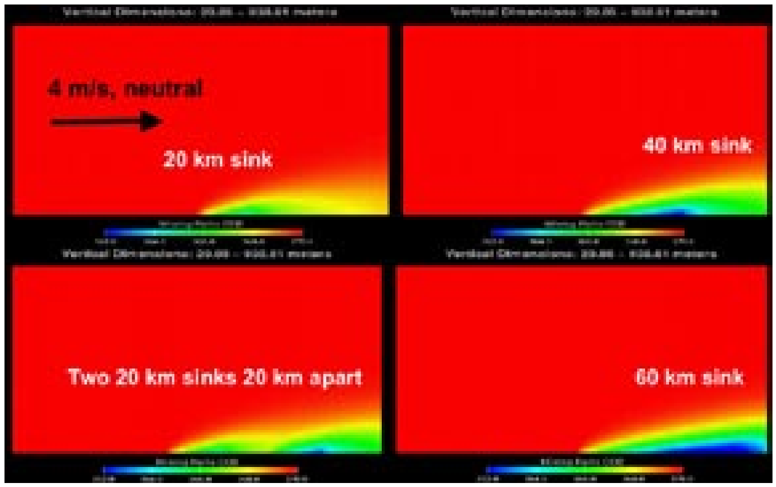
- Demonstrating rapid and large fractional removal of CO_2 from an air stream at gram-scale using alkaline solutions;
- Applying global scale and high-resolution atmospheric modeling to understand scale and scope;
- Examining the implications of direct air capture with respect to required scale;
- Estimating how the cost of capture justifies further research and development;
- Publicizing the concept to engage members of the research community.

Below: High-resolution modeling of CO_2 uptake flux as a function of sink size and separation. The panels show CO_2 levels as function of height and length for various size CO_2 sinks. The vertical scale is about 1 km and the horizontal scale is on the order of 100 km. The background atmospheric CO_2 levels are in red (370 ppm) and the losses caused by the sink are evident in the CO_2 distributions (blue indicates 362 ppm; green, 365 ppm; yellow, 368 ppm).

The Impact: Restoring the Atmosphere

Direct extraction of CO_2 from the air may prevent an increase in atmospheric carbon dioxide, and could possibly restore atmospheric CO_2 to pre-industrial levels. Direct air extraction of CO_2 also offers the following potential benefits:

- Controlling emissions from the myriad small CO_2 emitters that account for a significant share of global emissions;
- Providing purified carbon dioxide for use with a variety of storage options;
- Completely separating power generation and CO_2 capture processes in both space and time;
- Controlling CO_2 emissions from the transportation and home sectors without restructuring;
- Eliminating the need for extensive pipeline infrastructure to transport CO_2 from the source to the eventual sequestration sites.



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Integrated Approaches to Managing Terrestrial Carbon

The Challenge: Measuring and Mitigating Depletion of Terrestrial Carbon Pools

Managing terrestrial systems is a critical component of carbon management. Over the decades, terrestrial carbon pools have been depleted. The largest terrestrial carbon fluxes into and out of the atmosphere are caused by photosynthesis and respiration. Drought, fire, and other disturbances often result in large, rapid losses of terrestrial carbon. Current global carbon assessments do not quantitatively include such losses, and a scientific basis for doing so is lacking.

Los Alamos Innovation: New Approaches to Prediction and Management

To account for these losses, and to assess options for their mitigation where feasible, Los Alamos is using an integrated set of approaches. Los Alamos's assets include (1) advanced soil carbon measurement technology (Laser-Induced Breakdown Spectroscopy or "LIBS" and microbial biochemistry); (2) the CENTURY ecosystem modeling program; (3) field experimentation, including drought effects; (4) long-term monitoring; and (5) advanced carbon flux assessments.

Additional Los Alamos advantages in performing research on carbon in terrestrial ecosystems include

- The world's most instrumented semi-arid woodland site with the longest soil moisture data;
- A unique experimental facility for assessing drought impacts;
- Multi-tower assessment for estimates of high-resolution carbon fluxes while in progress;
- Detailed physiological data relating plant growth and mortality to soil and water;
- Linkages between vegetation pattern and soil erosion;
- A study facility with the world's most rapid change in an ecotone boundary (forest to woodland).

Combined with advances in soil carbon instrumentation, Los Alamos will have the ability to conduct rapid assessments and projections of carbon dynamics for different sites.

The Impact: Improved Ecosystem Management

Improving predictive capabilities and management strategies for carbon in terrestrial ecosystems could have far-reaching effects. Professionals in the field will be far better at predicting when plant mortality is likely to occur, how much erosion may result, what the impacts for carbon reserves will be, and how alternative management strategies would impact carbon stores. Terrestrial carbon pools could serve as important repositories for storing carbon and may help decrease carbon dioxide concentrations in the atmosphere.

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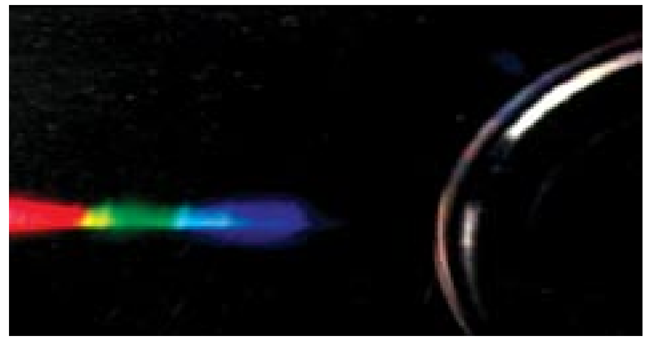
LIBS Analysis of Terrestrial Systems to Improve Carbon Management

The Challenge: Measuring Terrestrial Carbon Rapidly

Carbon fluxes into and out of terrestrial systems make up a significant share of the global carbon budget. Carbon management will likely soon include terrestrial sequestration, altering these carbon fluxes through active management of plant growth in forests, croplands, and woodlands. Tradable credits for sequestration are heightening interest in this approach. The key to market-based trading in terrestrial carbon sequestration is the ability to measure the quantity of carbon stored in soils, plants, and trees across diverse areas. There are drawbacks to current efforts to measure carbon in terrestrial systems; it remains both time consuming and costly.



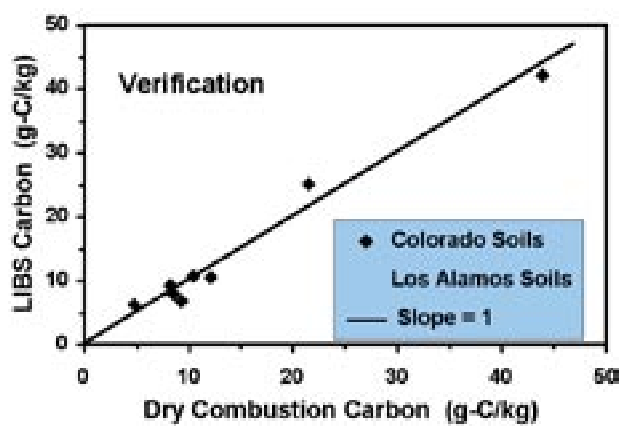
Los Alamos Innovation: Laser-Induced Breakdown Spectroscopy

Los Alamos originally developed Laser-Induced Breakdown Spectroscopy (LIBS) to analyze light elements in solids. Researchers have recently adapted this technique to the analysis of carbon in soils. LIBS analysis is particularly amenable to field-based carbon determination and to scenarios requiring rapid, almost instantaneous, measurement results at minimal cost. This instrumentation provides new analytical capabilities, including

- Rapid analysis (<1 minute per sample);
- Surface and subsurface measurements using a cone penetrometer system;
- *In situ* measurement with little or no sample preparation;
- Good sensitivity for carbon detection, with accuracy and precision rivaling laboratory methods;
- Simultaneous detection of other elements of interest.

With Laser Induced Breakdown Spectroscopy (LIBS), a laser produces a plasma which generates a color spectrum (above) characteristic of the elemental composition of the sample. This spectrum can be analyzed to determine carbon content, using conventional analysis methods to develop a calibration curve (below).

Laboratory efforts are now focused on applying LIBS to the rapid determination of carbon *in situ*. LIBS can be deployed in a number of analysis scenarios. Two transportable units are used to analyze discrete soil samples and to map in depth the carbon concentration in core samples. One unit is deployed at Los Alamos to monitor changes in soil carbon in ongoing programs, and a second unit is undergoing a nationwide U.S. Department of Agriculture testing program. Two-person portable units are in development to provide optimal field deployability for (1) verifying efficiency of sequestration protocols through direct soil analysis and (2) improving measurement (respecting both performance and cost) of soil carbon to elucidate heterogeneity in distribution.



The Impact: Improved Carbon Management

LIBS appears on its way to upgrading the measurment of carbon in terrestrial systems (particularly the speed and affordability) and strengthening programs for tradable credits in carbon sequestration. LIBS can play a key role in improving global carbon management.

Microbial Signatures to Monitor Soil Carbon

The Challenge: Detecting Early Changes in Terrestrial Ecosystems

Both the energy and agriculture industries could benefit from advanced tools for monitoring changes in soil carbon. The energy industry will need inexpensive carbon sequestration options, such as terrestrial sequestration, that will rely on carbon monitoring. Managing soil carbon is also critical to improving the efficiency of food production.

Los Alamos Innovation: Microbial Signatures for Soil Carbon

Los Alamos has initiated a project to use soil microbes as indicators of the status of soil carbon content and has succeeded in identifying the first set of microbial signatures of increasing, decreasing, and static soil carbon content. The size and diversity of microbial populations make them difficult to characterize. To simplify the problem, Los Alamos is focusing on specific genes in the microbial population and is creating modern DNA-based assays to examine the microbes in carefully selected target soils. Key Los Alamos efforts are directed toward (1) calibrating the microbial indicators on a few select soils and (2) testing several parameters for impact on the microbial population.

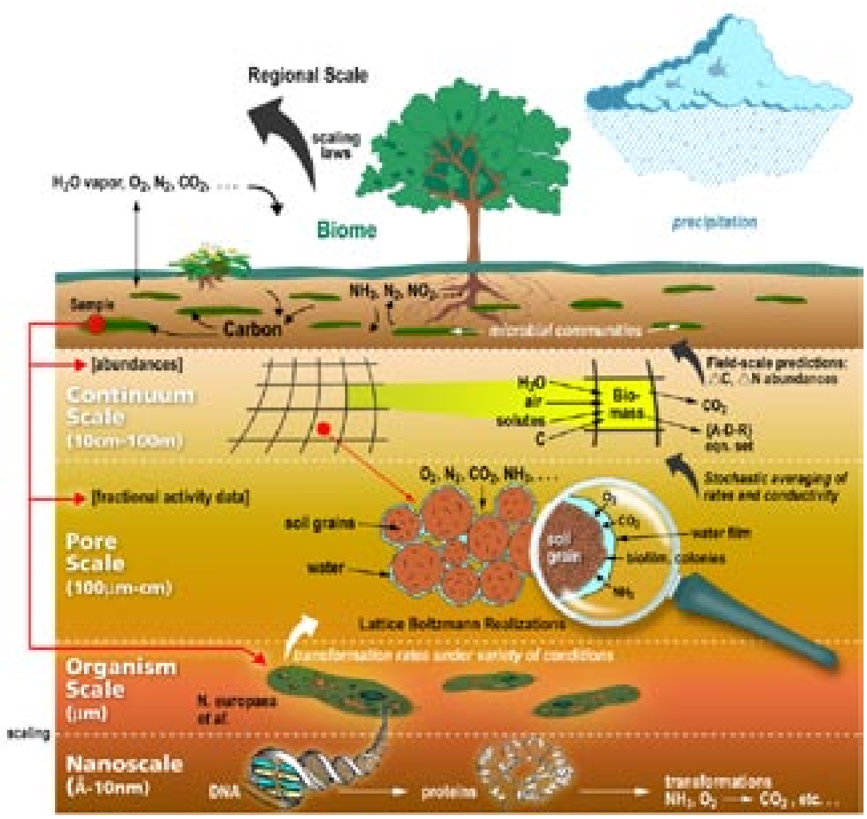
Building on initial success, the ultimate goal is to develop the microbial indicators into practical commercial tools for soil carbon monitoring. These tools could be applied to

- Detect increases in soil carbon early as an inexpensive assay;
- Forecast the permanence of carbon storage in soils by providing model data; and
- Assess soil productivity by providing data to parameterize models.

Microbial populations are integral components of the nanoscale systems that underpin terrestrial ecosystems.

The Impact: More Effective Terrestrial Carbon Management

Microbial indicators can be a valuable part of the suite of new monitoring technologies needed to indicate change in terrestrial ecosystems. Microbial signatures promise early, consistent, affordable, and highly predictive soil carbon monitoring. With these tools, the energy industry can meet higher environmental standards, and the agriculture industry can become more efficient and productive.



Los Alamos NATIONAL LABORATORY

An Integrated, Automated System to Process and Analyze Soil, Air, and Water

The Challenge: Effective Analyses of Soil, Air, and Water

To improve understanding of the carbon life cycle, analysis of large numbers of samples is needed. Traditional approaches to sample collection, tracking, preparation, and analysis are very labor- and time-intensive, and conventional techniques do not scale very well. A new system is needed to perform high-volume, rapid, reliable, and repetitious analyses of soil, air, and water.

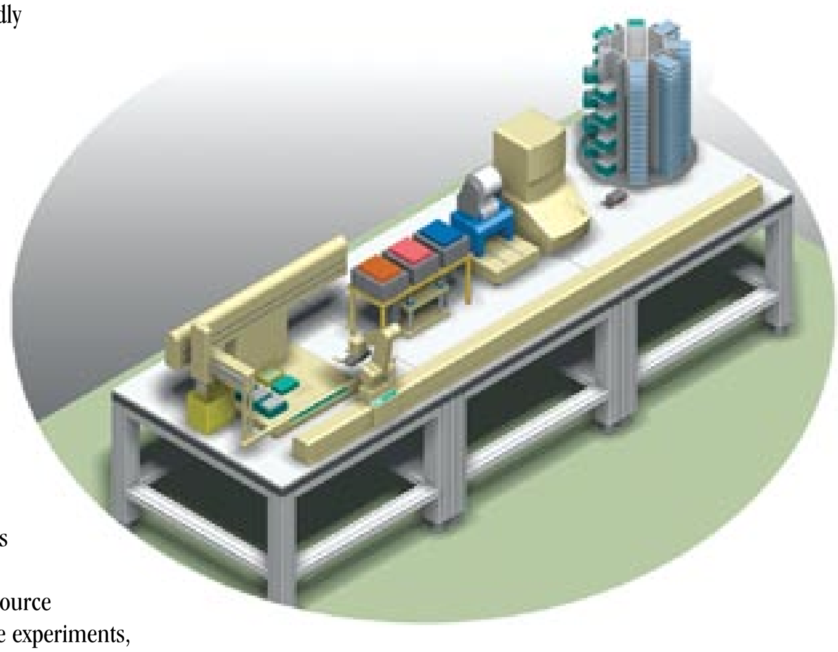
Los Alamos Innovation: Integrated and Automated Sample Analysis

The best way to achieve efficient, high-throughput sampling is by using an automated, highly-integrated sample processing and analysis system. To achieve this end, Los Alamos has formed a multidisciplinary team of biologists, chemists, mechanical engineers, software engineers, electrical engineers, and technicians. This team has considerable expertise in developing laboratory automation systems and custom instrumentation.

Working with industrial partners, other government agencies, and NIST, ASTM, and other standardization organizations, the Los Alamos team has developed equipment controls, interfacing standards, and systems that can be rapidly developed and deployed.

In the future, soil-sample processing systems could automatically separate, dry, pulverize, repackage, barcode, and weigh inhomogeneous soil samples. In addition to actively managing the sample material flow, this processing system would automate the information flow between all system components, thus enabling sample tracking and audit trailing.

An automated sample analysis system, which integrates sample processing, analysis, and tracking.



The Impact: Better Carbon Management

This system could be used to support soil sampling efforts ongoing at the U.S. Department of Agriculture and other research institutions. The benefits of automation technologies in carbon fuel cycle research and other research programs include (1) higher throughput, (2) lower costs, (3) more resource sharing, (4) automated result validation, (4) more repeatable experiments, (5) less potential for human errors, (6) more accurate results, (7) tracking, system monitoring, and reporting in real-time, and (8) reduced (possibly to zero) human exposure to potentially hazardous material environments. Processing samples automatically will reduce soil analysis costs and allow sufficient characterization of terrestrial systems for carbon management.

Los Alamos NATIONAL LABORATORY

Biophysical Principles and Models to Predict Biophysical Behavior

The Challenge: Predicting Biophysical Behavior

Predicting dynamics of terrestrial carbon systems and of biological systems generally is difficult but important. We lack a powerful underlying theory, and few universal biophysical principles are known beyond the genetic code and the evolutionary process. Across the size range from microbes to the biosphere, all life uses the same chemical constituents and reactions. All life functions by transforming energy from physical or chemical sources to build, maintain, and reproduce complex, organized structures and processes. How do we find the universal principles governing this immense variety of dynamic living forms, functions, and behavior?

Los Alamos Innovation: Predictive Biophysical Models

Los Alamos is addressing these issues and beginning to provide a quantitative basis for exploring biological systems and predicting their behavior. By extending current theory, conducting macro-ecological analyses, and conducting advanced experimental and observational testing, Los Alamos is producing and applying an integrated scientific capability.

Los Alamos scientists and collaborators have developed a model based on allometric scaling laws, which relate size to measurable biological quantities. This model quantitatively predicts and describes how energy production is constrained by the transport of resources in biological systems. So far, the theory has provided fundamental new insights related to terrestrial carbon, including in these five areas:

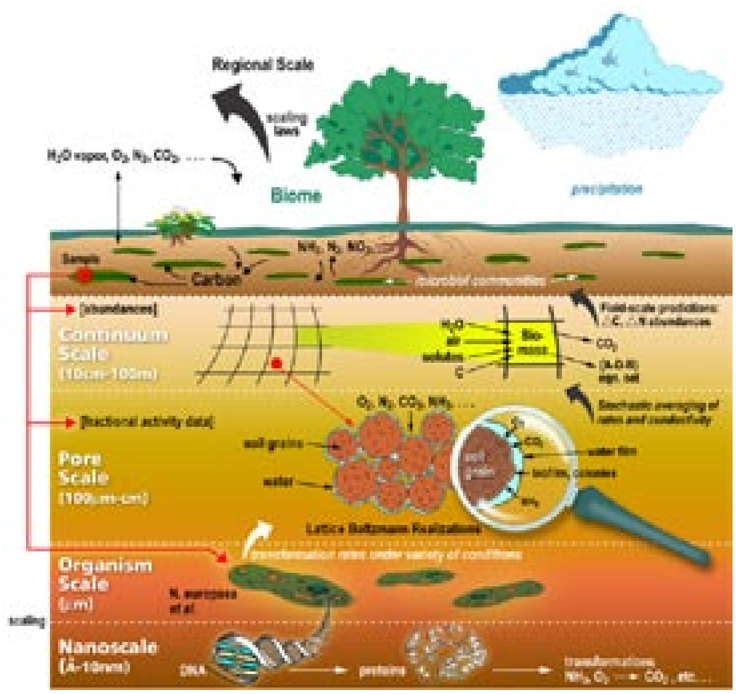
- Tree growth rates among diverse species;
- Above-ground vs. below-ground biomass;
- Biophysical constraints limiting tree size;
- Plant-spacing relationships; and
- Ecosystem photosynthesis, respiration, and associated carbon flux rates.

The Impact: Understanding Life at All Levels

Results suggest that this powerful new theory may be extended to offer a robust predictive and explanatory understanding of how biological energetics provides the basis for scaling, from molecules to the biosphere, and linking many attributes of biological structure, function, and diversity. The new theory will allow (1) broad-scale analysis of terrestrial carbon pools and dynamics across diverse ecosystems; (2) cost-effective assessments of terrestrial carbon sequestration options; and (3) improved predictive capability of trajectories of terrestrial carbon in a given system.

Understanding biophysical principles will not only improve carbon management, it will help us predict fundamental relationships and behaviors in biological systems. It can lead to understanding the nature of life at all levels.

Terrestrial ecosystems consist of processes and subsystems that function on scales ranging from the nanoscale to the biome scale.



GENIE Software to Monitor All Stages of the Carbon Cycle

The Challenge: Monitoring All Stages of the Carbon Cycle

Monitoring all stages of the carbon cycle—both natural and anthropogenic, and at various scales—is a continental-scale challenge. Monitoring includes detecting and measuring emissions from processing and storage facilities, and monitoring environmental state-of-health at natural and managed terrestrial sequestration sites. Remote sensing techniques (using both spacecraft and aircraft) are available, but involve mostly manual analysis. Traditional techniques are overburdened trying to keep pace with the flood of data from instrument platforms.

Los Alamos Innovation: GENIE Software to Assemble Remote-Sensing Tools

The solution: automated analysis techniques via modern machine learning methods providing adaptive, robust algorithms. The Los Alamos GENIE machine-learning software system uses a genetic algorithm.

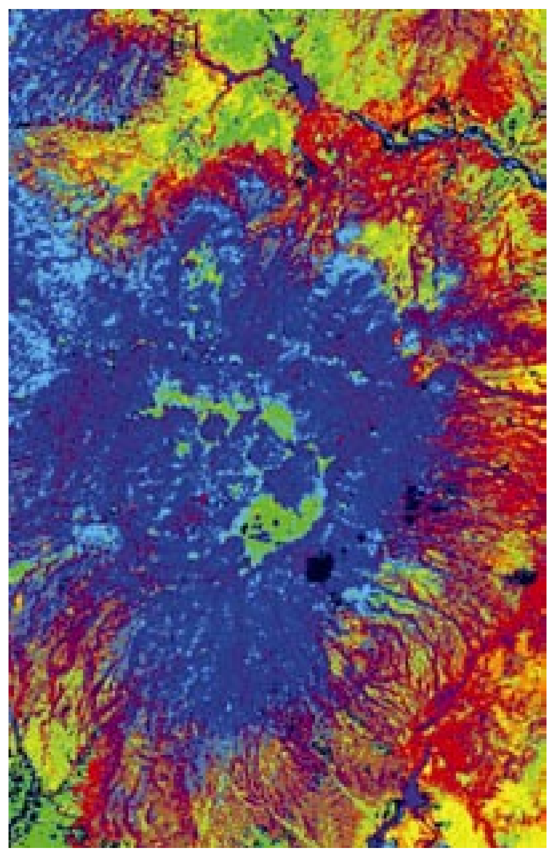
GENIE assembles automated remote sensing tools from low-level image operators. Each assembled tool is evaluated against training data provided by the user, and the best tools in each generation are allowed to reproduce to build new tools. The population of tools evolves until it converges to a solution or reaches a minimum level of performance specified by the user.

GENIE provides the capability to build a suite of robust, adaptive tools to detect and analyze problems at production and storage facilities and terrestrial sequestration sites. In the future, GENIE will be used to rapidly prototype and field remote-sensing algorithms customized for automated monitoring. Tools will be developed capable of fusing and exploiting new and archival data from satellite and aircraft instruments (including advanced sensors such as multi-spectral and synthetic aperture radar imagers).

The Impact: Mapping Effects of Disasters and Carbon Cycle Monitoring

Already GENIE has been applied to a range of real-world problems. GENIE mapped the effects of the 42,000-acre Cerro Grande wildfire in Los Alamos in May 2000. And, using satellite and aircraft optical and multi-spectral imagery, GENIE helped detect ash, debris, and the plume from the terrorist attack in New York City on September 11, 2001. In the future, GENIE will be used to develop tools for many more real-world applications. GENIE promises to help achieve monitoring of all stages of the carbon cycle.

GENIE land-cover map for the Jemez Mountains, NM, using a Landsat satellite image. GENIE was trained to find trees, grasslands, and bare soil using a small, manually produced map, and then asked to automatically remap an area hundreds of times larger. These results support forest state-of-health monitoring, wildlife habitat assessment, and wildfire emergency response planning.



Microhole Drilling and Diagnostics to Contain Subsurface CO_2

The Challenge: Ensuring Containment of Subsurface CO_2

Ensuring that $C0_2$ is contained is a critical aspect of geologic sequestration. With conventional drilling, it is considered cost prohibitive to deploy sufficient instruments to adequately monitor sequestration processes.

$C0_2$ containment is ensured by measuring chemical and physical processes in the subsurface rock surrounding the new CO_2 reservoirs. To place the measuring instruments in the subsurface requires drilling. Contemporary deep boreholes have relatively large diameters. Advances in electronics and sensor miniaturization in the past decade have made new instrument packages with small diameters possible and increasingly affordable. These instrument packages, however, are poorly suited for large boreholes. Advanced drilling technologies are required to drill small-diameter boreholes primarily for deploying subsurface instrumentation.

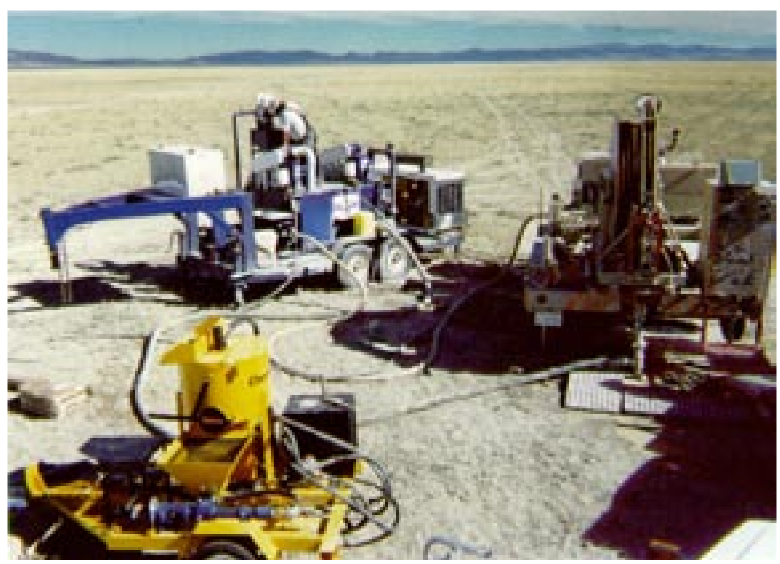
Los Alamos Innovation: Microhole Drilling and Diagnostics

Los Alamos is developing microhole technologies for use in boreholes. These coiled-tubing technologies eliminate handling of segmented large-diameter drill pipes. Microholes with diameters of 2-3/8 and 1-3/4 inch are currently being drilled. With decreased size and use of materials to drill and complete microholes for instrumentation, savings of nearly 60% (discounting labor savings) will be realized.

Borehole instruments with 7/8-inch-diameter housings have also been developed and successfully deployed in microholes. To date, most of the advances in instrumentation have been in the area of microseismic instrumentation, used to detect subtle movements in fracture-dominated rock masses. Exploratory studies have revealed no engineering impediments to developing electrical-resistivity or nuclear-fluid monitoring tools for deployment in these wells.

The Impact: Better CO_2 Containment at Lower Cost

Microhole technology can reduce the cost of deploying instruments in the subsurface while improving measurement quality. This can greatly enhance safe CO_2 containment at geologic sequestration sites.



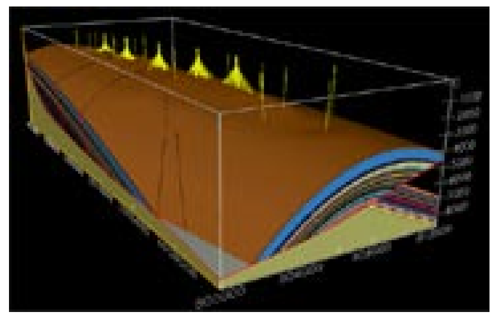
Microhole coiled-tubing drilling rig deployed in central Nevada for drilling cased 1.25-inch diameter microholes for emplacement of seismic instrumentation. The tan equipment is the coiled tubing drilling rig, the blue is a mud conditioning system, and the yellow is a PVC casing grouting system.

Investigative Modeling to Predict the Fate of Injected CO_2

The Challenge: Safely Storing CO_2 in Geologic Reservoirs

Large volumes of CO_2 can be sequestered in depleted oil and gas reservoirs, deep saline aquifers, deep unmineable coal seams, and similar geologic sites. Long-term storage of CO_2 in geologic formations would result in reactions between the CO_2, groundwater, and the geologic media. The reactions would change properties of the storage environment. This could affect the integrity of the natural barriers and could result in release of CO_2 to the accessible environment, adversely impacting health and safety.

Enhanced oil recovery methods have shown that large amounts of CO_2 can be injected into depleted oil reservoirs, but these methods have a short application history (about 50 years). Only with the capability to verify geologic sequestration methods with accurate predictive modeling tools will such long-term storage of CO_2 be possible.



Los Alamos Innovation: Investigative Modeling of Injected CO_2

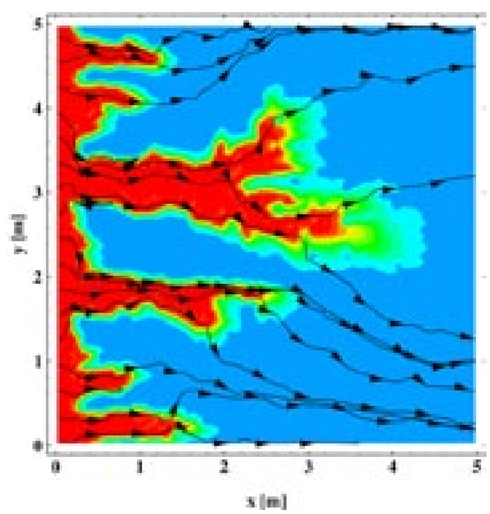
With new models, especially those coupling earth processes, it is possible to assess the fate of CO_2 injected into geologic formations. Los Alamos's numerical codes can be used to model the multiple, complex interactions of CO_2 and minerals in geologic media. While studying geothermal energy reservoirs, Los Alamos researchers developed numerical models for coupled heat-flow-mass transfer problems. These models have since evolved to study flow and reactive transport of contaminants in aquifers. Key abilities of these models include

- Coupling the heat-flow-mass transfer approach;
- Modeling problems that result in reactions with porous media; and
- Integrating EOS and reaction table data with an extensive thermodynamic application range.

Predicting the fate of CO_2 in the subsurface over time requires integrating reservoir-scale models (above) with detailed simulations of physical and chemical processes at the pore scale (below).

The Impact: Predicting the Long-Term Fate of CO_2

Predicting the geologic fate of CO_2 has many applications, particularly in predicting CO_2's fate in sites considered for carbon sequestration. These models have been extensively applied to determine the fate of contaminants for a large number of contaminated sites in the vicinity of Los Alamos. In addition, they have been used to determine the long-term safety of the Yucca Mountain high-level nuclear waste repository. Long-term dynamic simulations could be used to understand how CO_2 and geologic media would interact over geologic time frames. Ultimately, it may be possible to predict how storage of CO_2 will affect the geologic media and the long-term safety and feasibility of geologic sequestration.



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Magnesium-Silicate Mineralization for Permanent Storage of Carbon Dioxide

The Challenge: Long-Term Storage of CO_2 Emissions

Each year, fossil-fuel use in the U.S. produces twenty tons of CO_2 per person. Worldwide, total emissions now exceed twenty billion tons per year—5 cubic miles in liquid form. By the year 2099, these emissions could easily increase by a factor of 5 to 10 times. These enormous volumes will impose significant constraints on potential storage options.

Los Alamos Innovation: Converting CO_2 to a Solid Carbonate

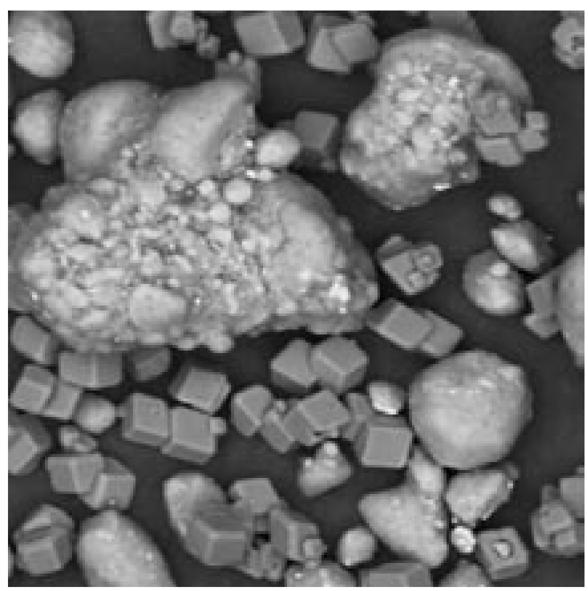
The ability to store large volumes of CO_2 safely for extended periods of time (thousands of years) is critical. Most of the CO_2 that once dominated the Earth's atmosphere has been removed by a natural process that weathered silicate materials to produce dissolved carbonates, clay minerals, and solid carbonates. Through this process, nature has safely stored much more CO_2 than could be produced by all of the world's fossil fuels.

Los Alamos researchers proposed an analogous approach to store anthropogenic CO_2 as a stable solid. Los Alamos proposed that serpentinites and other magnesium-rich silicate deposits could be reacted industrially with CO_2 to form silica and magnesium carbonate, resulting in a safe and immobile long-term storage medium for carbon dioxide.

In an effort funded by the National Energy Technology Laboratory (NETL), Los Alamos has partnered with several organizations to understand the conditions necessary for CO_2 mineralization and the processes that control its rate. The emphasis of the research is to identify a process that will allow CO_2 mineralization at a rate and cost that make it competitive with more conventional approaches to CO_2 sequestration.

Conversion is possible in an aqueous process, but sufficient rates are only achievable with limited olivine-rich ores and extensive (and costly) mineral preparation (mechanical grinding or heat treatment). Los Alamos's current process is most rapid at elevated CO_2 pressures (>1000 PSI), but pressures as low as 150 PSI appear encouraging.

Scanning electron microscope image of magnesite (rhombs) formed by reacting supercritical carbon dioxide with the magnesium silicate serpentine.



The Impact: Safe Permanent CO_2 Storage

Benefits of this process include

- Safety—magnesium carbonate is benign and has no negative impacts on the environment;
- Immobility—solid magnesium carbonate requires no long term monitoring and provides easy verification of storage volumes; and
- Valuable by-products—serpentinites and many other magnesium-rich rocks are enriched in platinum group elements and other valuable metals.

If a feasible, economic process can be developed, CO_2 mineralization could be implemented with any capture process that provides a relatively pure CO_2 stream.

Ocean Simulations to Predict Effects of Carbon Management Plans

The Challenge: Understanding How Iron Affects the Ocean

The deep ocean is the largest potential CO_2 reservoir accessible from the Earth's surface. Over the next few centuries, the ocean will serve as a natural sink for atmospheric greenhouse gas. It is thought that engineering changes in micro-nutrient iron supply to oceanic plankton would significantly effect concentrations of atmospheric CO_2. Implementing large-scale iron fertilization to alleviate greenhouse gas is fast approaching economic viability. However, the fate and effects of this injected material would influence the ecology of the ocean. To understand the potential risks, advanced new tools are needed.

Los Alamos Innovation: Simulating Oceanic Carbon Cycles

A detailed ocean biogeochemistry model has been under development at Los Alamos. It includes many nutrients, tracers, and other metrics that influence the carbon cycle. The simulations are built into and based on the global general circulation models for which the Laboratory's climate team has become well known. Los Alamos codes can produce high resolution of biological and elemental cycling while supporting full biogeochemistry. Carbon related issues being addressed in the model include

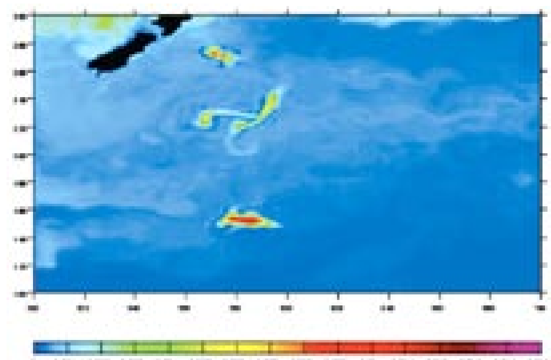
- Observing the impact of El Niño/La Niña events on marine ecosystems;
- Mimicking the behavior of patches created during the Southern Ocean Iron (Fe) experiments (SOFeX);
- Identifying oceanic regions where sequestered CO_2 might return to the surface rapidly; and
- Performing detailed simulations of the behavior of proposed iron fertilization of the oceans for carbon sequestration.

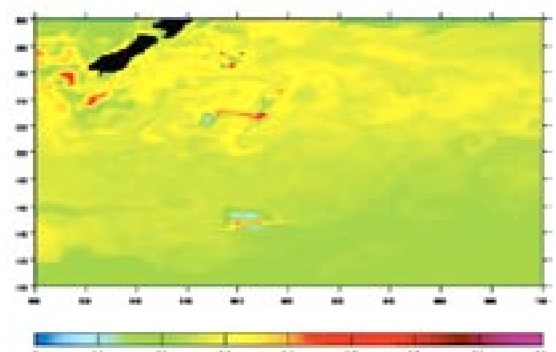
In the future, Los Alamos will investigate (1) how spatial and temporal dispersion of sequestered carbon can be predicted after perturbation; (2) how adding micro-nutrient iron to the surface ocean would stimulate marine organic carbon production; (3) how much organic carbon will sink to the deep ocean and to what extent it will be replaced by atmospheric CO_2; and (4) how iron fertilization changes physical and chemical conditions (both on the surface and mid-water).

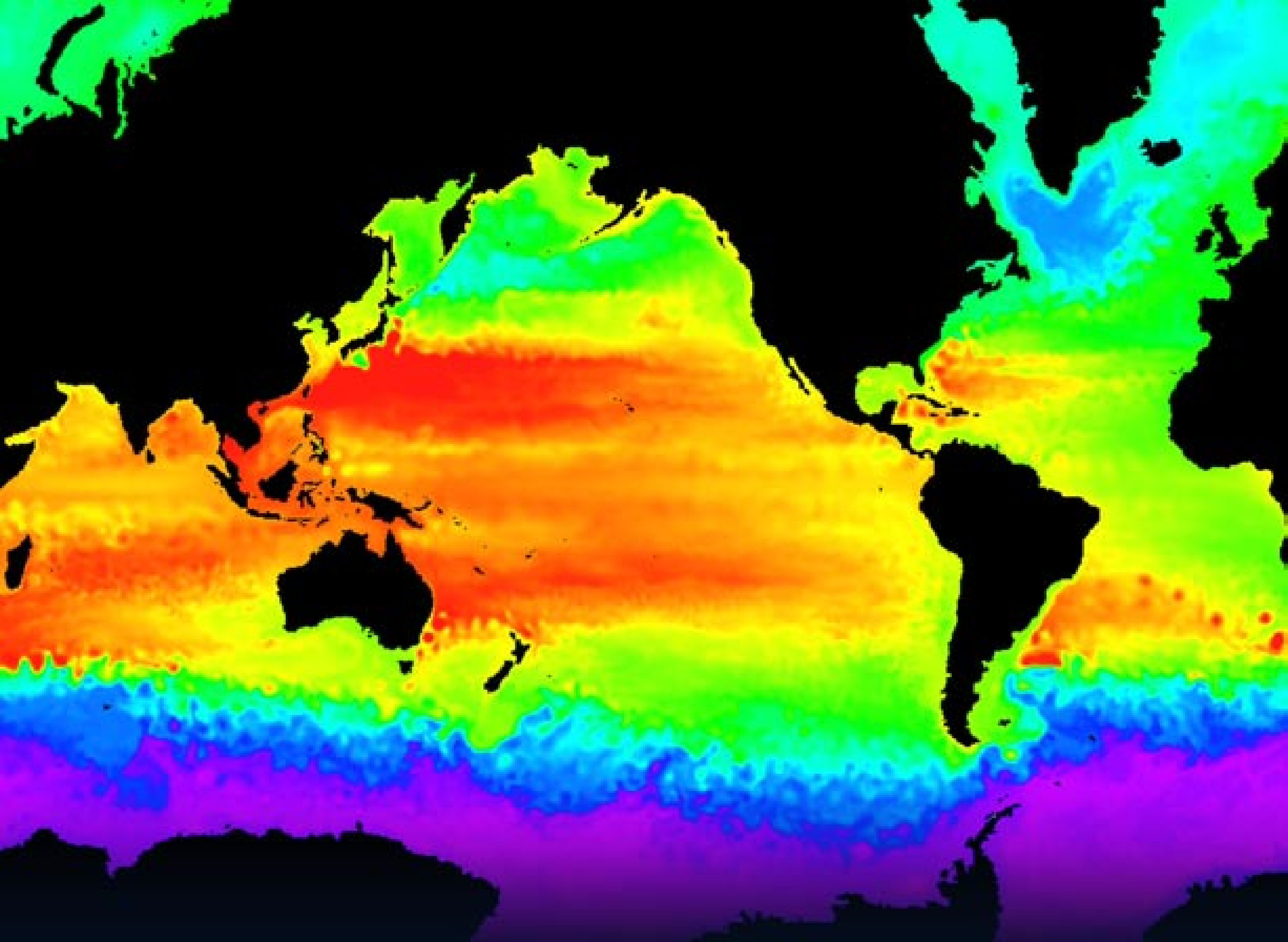
The Impact: Knowing If Iron Can Safely Reduce Greenhouse Gas

Los Alamos's ocean-carbon sequestration studies will show how proposed marine carbon management plans affect the long-term fate of ocean environments. Enabling evaluation of various ocean sequestration strategies could have major implications for environmental management. If it is found that fertilizing the ocean with iron will have minimal effect on ocean ecosystems, policymakers may decide this is a viable solution for reducing or alleviating greenhouse gas, holes in the ozone, and global warming.

Biogeochemical model of three iron-enrichment patches introduced south of New Zealand. Iron is introduced in the model as roughly one-nanomolar iron injections over three square areas, each approximately 100 km on a side. The top image shows the resulting distribution of iron after one month of processing by surface ocean biology transport. The second image is the corresponding phytoplankton distribution (units of micromolar plant nitrogen content). Strong biological growth is apparent in the fertilized areas.







CLIMATE

Energy and Environment Compendium

Los Alamos
NATIONAL LABORATORY

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Climate Research at Los Alamos National Laboratory

Climate Research at Los Alamos National Laboratory

Climate variability presents a range of challenges to the future well-being of society. The prospect of global warming due to increasing greenhouse gases will impact environmental cycles and energy planning in highly uncertain ways. Improving our understanding of these impacts and developing adaptation and mitigation strategies is a national problem that Los Alamos is addressing.

Sound energy policy requires an understanding of the primary external drivers that will impact the nation's energy future over the next 25 to 50 years. One of the principal impacts is from climate variability induced by both natural cycles and anthropogenic forcing. To prepare for this looming issue, the collective resources of the Department of Energy's national laboratories will be necessary to develop innovative strategies that can ensure the success of the DOE in its energy security mission.

Los Alamos has developed a full range of capabilities to address the problem of climate variability. The foundation of these capabilities resides in our world-renowned program in global ocean modeling. These ocean models are a primary component of the nation's foremost climate prediction system. Climate process models have also been developed at Los Alamos and implemented into our ocean models to investigate ocean carbon cycling. At the regional scale, Los Alamos has an ongoing effort that has made great strides in developing a comprehensive model to predict water resources within the upper Rio Grande Basin. The Laboratory also operates and maintains three climate monitoring sites in the Tropical Western Pacific for the DOE's Atmospheric Radiation Measurement (ARM) program.

Current Scientific Challenges in Climate Research

Improved Prediction—Additional ocean and terrestrial data sources from remote sensors and climate monitoring stations are required to validate coupled global climate models that are undergoing continuous improvements to achieve higher resolution and more accurate representations of climate processes.

Regional Climate—It is necessary to understanding climate change impacts on human infrastructures and ecosystems over specific geographical regions where policy is implemented. Reducing the uncertainty in regional climate variability predictions is key to adapting to and mitigating climate change effects.

Aerosols—Anthropogenic aerosols are the most uncertain component of climate variability prediction due to their feedbacks on the radiation balance of the climate system. Recent research indicates aerosols may also be implicated in the suppression of hydrologic cycles over regions of the globe.

Decision Models—Achieving better understanding of global to regional climate variability and its feedbacks throughout the geophysical system will lead to improved forecasts and assessments. These can be developed into decision support systems that can determine climate change impacts on the human condition and help to reduce the costs of adaptation and mitigation.

Problem-Solving Capabilities in Climate Research

Los Alamos maintains and continues to develop climate-related research and development capabilities in the following areas:

Modeling and Simulation
- Global Ocean
- Parallel Ocean Program (PoP)
- Miami Isopycnal Ocean Model HYCOM/MICOM
- Sea Ice—CICE model
- Numerical and Gridding Methods
- Massively Parallel Computing Applications
- Regional Climate Modeling—RAMS/LADHS

Climate Processes—Modeling and Measurements
- Ocean Biogeochemistry
- Water Resources/Hydrology
- Atmospheric Aerosols
- Radiative Transfer
- Atmospheric Chemistry
- Terrestrial/Marine Ecosystems
- Wildfire Behavior
- Hurricane Intensity Prediction

Climate Monitoring
- ARM—Tropical Western Pacific climate stations
- Ecological monitoring of semi-arid landscapes
- FORTE/GPS—lightning data to global scales
- Image Analysis—GENIE software

Paleoclimate
- Isotopic correlation with dendrochronology
- Ecohydrology applications

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In addition to Los Alamos's extensive capabilities in modeling and monitoring the physical environment, the Laboratory is also recognized for its capability in energy infrastructure modeling for the Department of Energy and Department of Defense. These models require realistic inputs of economic and population dynamics in addition to data from a comprehensive model of the behavior of the future physical system. These inputs are used to drive realistic scenarios of energy demands. Combining our capabilities in understanding the physical, infrastructure, and economic environment can provide a unique capability to address future threats to energy security from climate variability and demographic shifts.

Climate, Ocean, and Sea Ice Modeling Project

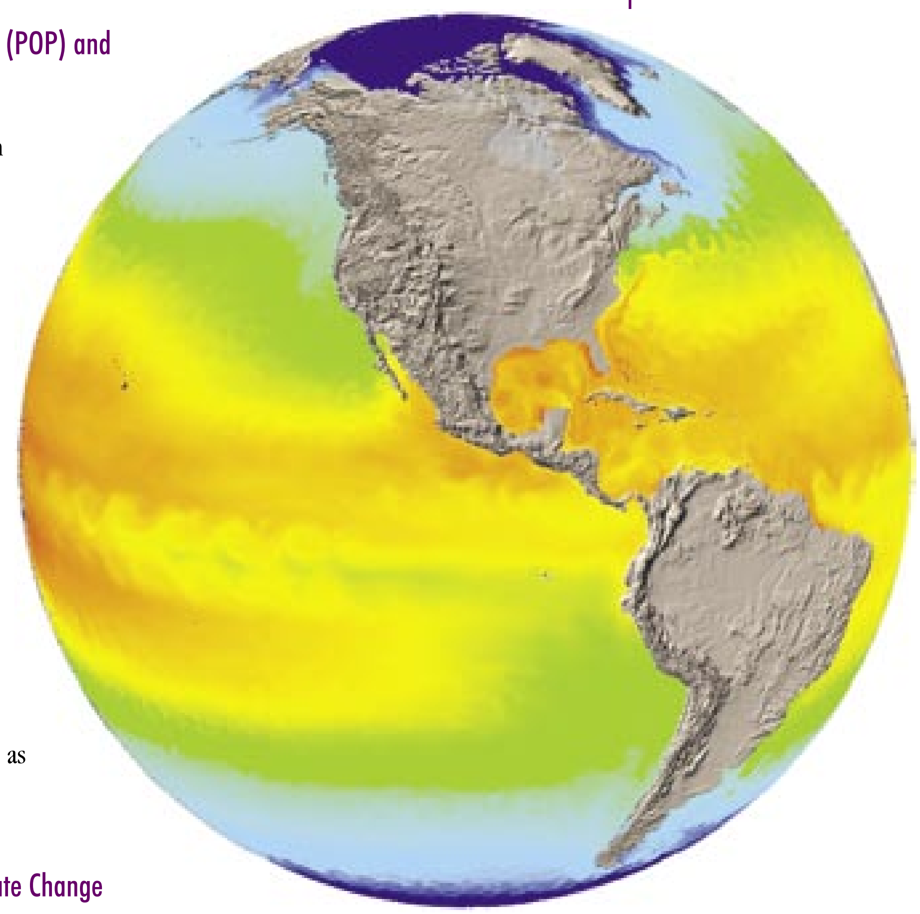
The Challenge: Understanding the Role of Oceans and Sea Ice in the Climate System

The primary mission of the Climate, Ocean, and Sea Ice Modeling (COSIM) project is to improve our understanding of the ocean and sea ice and their roles in the climate system. It has been designated by Los Alamos National Laboratory as a model development center under the Department of Energy Climate Change Prediction Program. In collaboration with other institutions, COSIM researchers have joined ocean and sea ice components with atmosphere and land components for fully coupled models of the Earth's climate system. The models are used for national and international climate assessments, including decadal-to-centennial climate change.

Los Alamos Innovation: Parallel Ocean Program (POP) and Sea Ice (CICE) Models

Developed at Los Alamos by a multidisciplinary team of physical scientists, applied mathematicians, and computer scientists, the POP and CICE models have been publicly released and used throughout the world's climate community. They also form the ocean and sea ice components of the Community Climate System Model (CCSM), a community modeling effort based at the National Center for Atmospheric Research.

In addition to these high-profile successes, the Laboratory's high-performance computing capabilities have enabled COSIM researchers to develop and validate physically and computationally advanced codes for simulating the circulation of the world's oceans, including the cryospheric component. Ultra-high resolution POP simulations of ocean circulation have also been performed and these simulations have been used to improve the understanding of the ocean and sea ice, as well as their role in the climate system.



Sea surface temperature from a high-resolution (1/10 degree) simulation of global ocean circulation using the POP model.

The Impact: Accurate Simulation of Global Climate Change Scenarios

The global modeling expertise and experience gained from the COSIM project and its participation in community modeling have resulted in the successful link of the wider global climate community with access to community data sets and other component models. The project has also provided valuable tools that can be used to directly simulate global change processes and scenarios. Data to drive other models, such as regional downscaling studies, have also been provided. In addition, the physical fidelity and computational performance of POP and CICE have continually been improved and have allowed for greatly enhanced ocean simulations for climate change scenarios.

High-Resolution Ocean Simulations

The Challenge: Developing a High-Resolution Simulation of Ocean Circulation

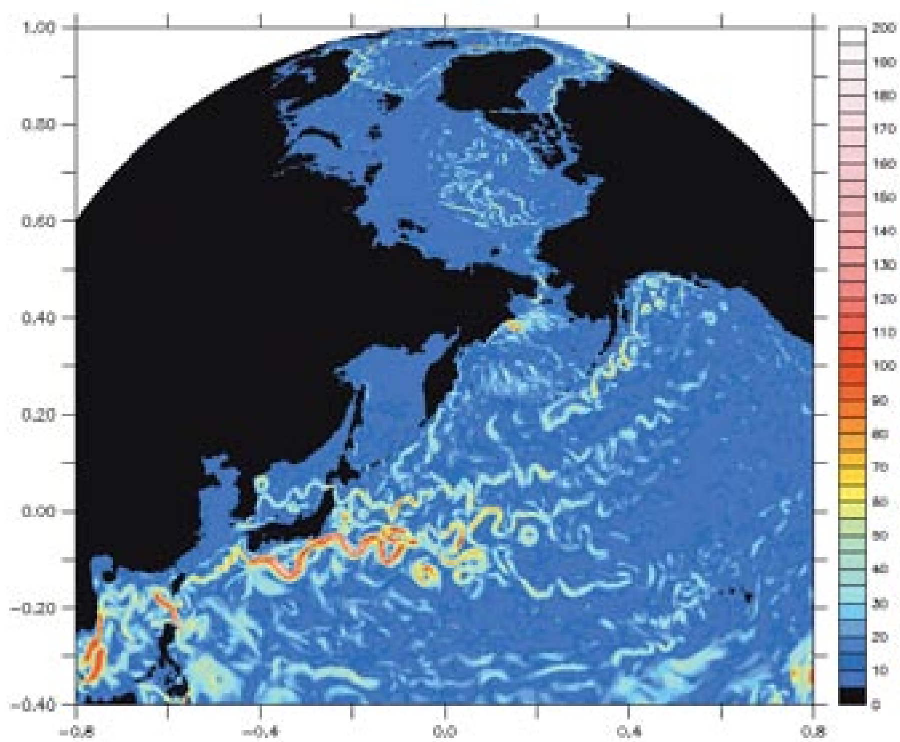
The Los Alamos Parallel Ocean Program (POP) in applied environmental prediction has long been considered for use by the U.S. Navy for acquiring high-resolution simulations of ocean circulation. POP allows Los Alamos to provide simulations of the ocean's circulation at a very high resolution (1/10th degree grid spacing). This simulation would then be used as an initial condition for short time scale ocean atmosphere predictions in regions of strategic interest to the Navy.

Los Alamos Innovation: High-Performance Computing for High-Resolution Simulations

Los Alamos National Laboratory's Climate, Ocean, and Sea Ice Modeling (COSIM) project is known for its use of high-performance computing to perform high-resolution simulations of ocean circulation. It is this expertise that has separated Los Alamos from other institutions and led to its selection by the U.S. Navy to perform ocean circulation simulation. This simulation was the largest ever attempted using a coupled model and fit successfully into the potential progression of runs. Preliminary results from this simulation have demonstrated that POP is capable of being used as a member of a predictive coupled model.

The Impact: Improved Ocean Models

Undertaking the ocean circulation simulation project has helped the COSIM project to improve ocean models, further augmenting the Laboratory's capabilities in modeling climate. It also reinforced Los Alamos's belief that high-resolution simulations play a crucial role in understanding ocean circulation. Such successes will allow the Laboratory to continue to perform these kinds of massive runs for a diverse clientele. This includes coupling with sea ice at high resolutions in order to create higher fidelity solutions in polar regions.



A snapshot of the current speed (cm/sec), at a depth of 15 meters, from a 1/10th degree POP ocean circulation simulation, reveals realistic features. Shown here is the meandering Kuroshio Current off Japan's East coast with its turbulent nature.

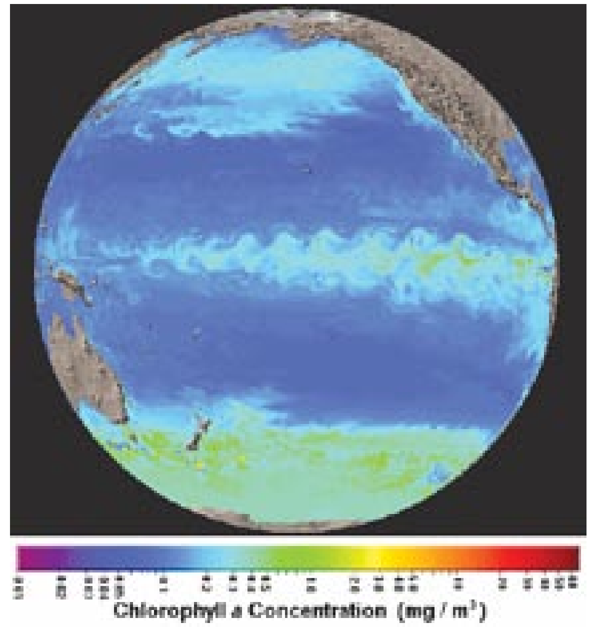
Biogeochemistry

The Challenge: Anticipating Threats Posed by Climate Change

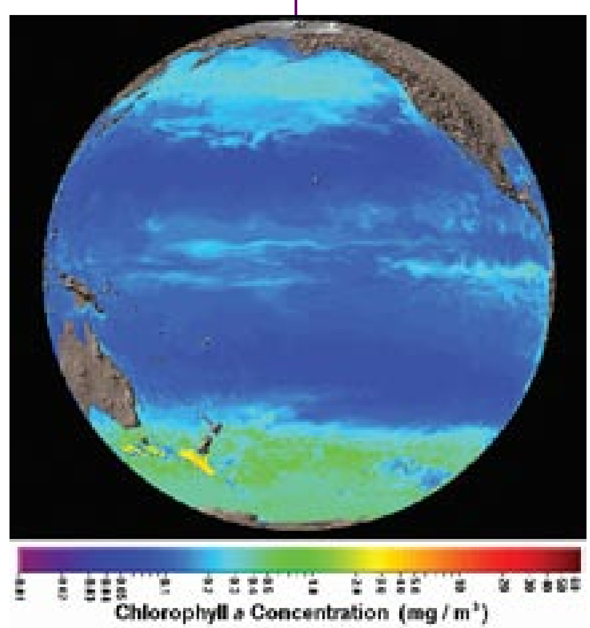
Current U.S. environmental policy emphasizes comprehending global change and developing technological solutions to the immense problems posed by greenhouse warming. The national climate science community and its Department of Energy component have responded to this by supporting detailed earth system modeling and simulation. These efforts include modeling of climate physics, basic elemental cycling within the coupled ocean atmosphere system, strategies for carbon management, and other aspects of global biogeochemistry.

Los Alamos Innovation: High-Resolution Ocean Biogeochemistry Modeling

The Los Alamos ocean modeling team has successfully introduced biogeochemistry routines into its Ocean General Circulation Model (OGCM). Los Alamos's approach to ocean biogeochemistry modeling is unique in several crucial ways. Most importantly, the simulations are built into and based upon the fine mesh global general circulation models for which the Laboratory climate team has become well known. Biology and elemental cycling in the upper ocean are tightly coupled to vertical pumping by horizontal eddies at the 10 to 100 kilometer scale. Only Los Alamos's codes are capable of producing this sort of resolution while also supporting full biogeochemistry. The model has been used to study the impact of El Niño/La Niña events on marine ecosystems and to create detailed statistical simulations of the behavior of proposed iron fertilization of the oceans for carbon sequestration. Also included is the coupling of marine mixed layer trace gas mechanisms with processing by tropospheric chemistry modules and intercomparison of surface ocean ecodynamics models.



Results from an eddy resolved simulation show the impact of El Niño/La Niña on the marine ecosystem: surface chlorophyll distribution in late 1996 (top figure, La Niña year), and late 1997 (bottom figure, full El Niño conditions).



The Impact: Knowledge to Form a Marine Carbon Management Plan

Los Alamos's ocean biogeochemistry studies will allow researchers to investigate the coupling of Earth's climate and biogeochemical systems and to study possible linkages and feedbacks occurring between ocean physics, biology, and chemistry. The studies will further help clarify the costs, benefits, and environmental ramifications of marine carbon management plans. Further improvement of carbon cycling within the Community Climate System Model is also a primary goal of this effort.

Global Ocean Modeling with the Hybrid Coordinate Model (HYCOM)

The Challenge: Reducing Uncertainty in Long-Term Climate Prediction

To reduce uncertainty in long-term climate prediction, the Intergovernmental Panel on Climate Change (IPCC) relies on multi-model ensemble forecasts made by pooling the world community's stock of climate models. However, the IPCC is well aware that, since these models were not developed independently of one another, "such an ensemble does not constitute an independent unbiased sampling of possible model formulations." Until recently, the climate model "gene pool" has been particularly sparse with respect to its oceanic component.

Los Alamos Innovation: Expanding the Ocean Model Base with Hybrid Coordinate Models

Responding to this situation, Los Alamos's Climate, Ocean, and Sea Ice Modeling (COSIM) team several years ago decided to broaden its ocean model base from one to four, essentially by adding an isopycnic-coordinate model, MICOM, to the in-house Cartesian coordinate model (the Parallel Ocean Program, or "POP") and by using both as the basis for developing so-called hybrid coordinate models. The principal design difference between Cartesian and isopycnic ocean models is that a Cartesian model treats depth as an independent variable and water density as a dependent variable, whereas an isopycnic model switches the role of the two. While the underlying dynamic principles are not affected by this switch, the differential equations describing the laws of fluid dynamics are noticeably different, particularly in their computer-solvable finite-differencing methods. Hybrid coordinate models (HYCOM's), viewed by many as an important and much-anticipated step toward the "ultimate" ocean model, attempt to combine the advantages of isopycnic models in the deep ocean (where water parcels move along density surfaces) and of Cartesian models in the surface mixed layer (where turbulent exchange processes are best modeled in a framework of constant-depth surfaces).

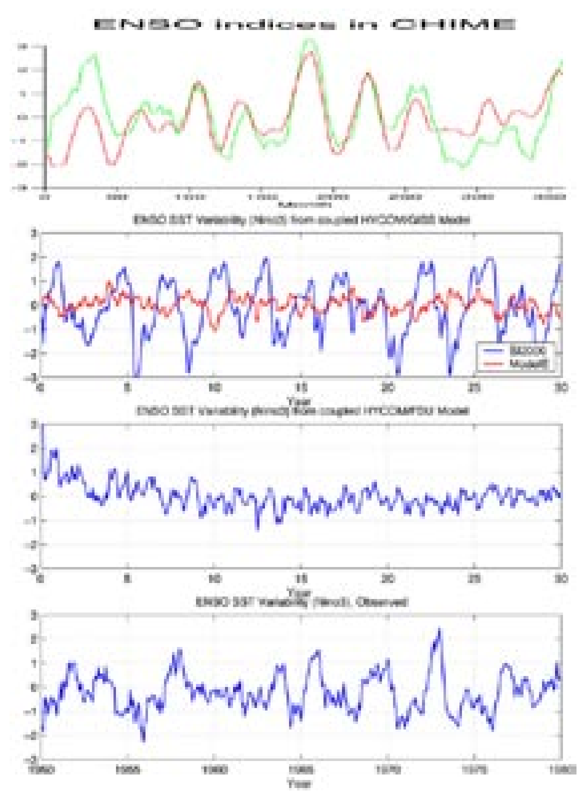
By providing three ocean model architectures, Los Alamos National Laboratory is unique among the world's climate research centers. This diversity has spawned within the COSIM team the development of diagnostic software allowing detailed, process-oriented intercomparisons of model results. Current process studies focus on the way our different models maintain the meridional overturning circulation (MOC) in the world ocean in response to changes in surface forcing (e.g., during global warming). The MOC is believed to be one of the more fragile links in the global heat distribution system, and our ability to predict the climate on multidecadal time scales depends critically on our models' abilities to mimic the natural variability of the MOC.

The Impact: More Accurate Climate Change Planning

Los Alamos's HYCOM/MICOM modeling efforts will

- Participate in the current round of IPCC assessments of the likely effect of CO_2 doubling on the earth's climate;
- Investigate the resiliency of the MOC during global warming and regional consequences of a possible breakdown;
- Simulate the carbon cycle with emphasis on enhancing oceanic CO_2 sequestration via iron fertilization; and
- Assess regional impacts of greenhouse-gas-induced global change.

Thirty-year time series of El Niño-related sea surface temperature variability (°C) in HYCOM coupled to several atmospheric circulation models. Different colors indicate model runs based on different parameter choices. The large model-to-model variation in Niño3 amplitude is largely unexplained and the subject of intense research.



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Los Alamos NATIONAL LABORATORY

Collaborative Development of the Community Climate System Model

The Challenge: Developing a Community Climate System Model

Community Climate System Model (CCSM) developers at Los Alamos are working on software design, performance optimization and portability, and model development. The ultimate goal of the project is to enable the addition of atmospheric chemistry and ocean biogeochemistry to the coupled model. Under the DOE Scientific Discovery through Advanced Computing (SciDAC) program, an effort was funded for the collaborative development of CCSM for terascale computers. The SciDAC collaboration includes Los Alamos and five other DOE laboratories, the National Center for Atmospheric Research, and the NASA Data Assimilation Office.

A computer model of the Earth's climate system is made up of individual computer models for the four main components: the atmosphere, the global ocean, sea-ice in the polar regions, and the land surface. These components interact by passing information to each other through a "coupler." If atmospheric chemistry and ocean biogeochemistry are included, the carbon cycle of the Earth can be studied. Each of the component models is designed to run on multiple processors, and all components also run in parallel on different processor sets on a single massively parallel computer.

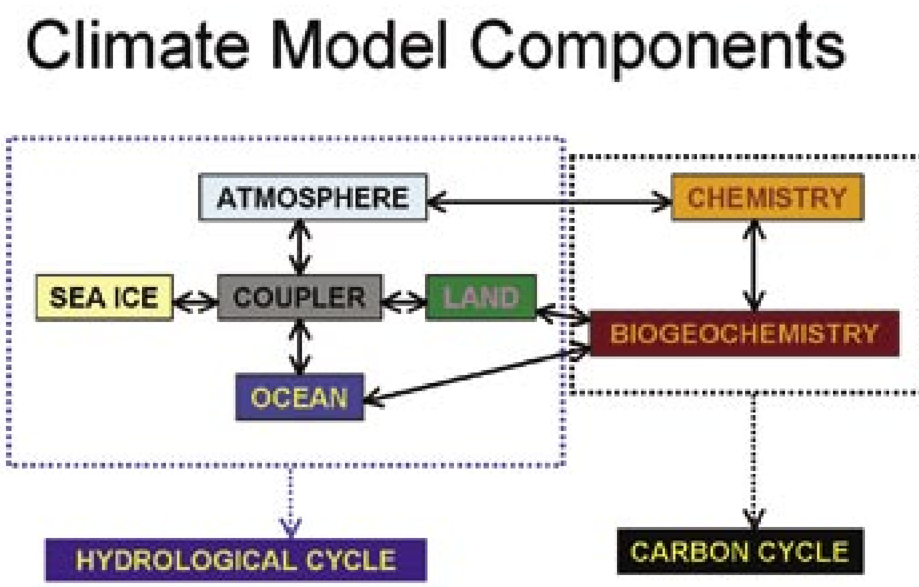
Los Alamos Innovation: Enhancing All Aspects of the CCSM

With expertise in high-performance computing and collaborative software development, Los Alamos's role in SciDAC has improved the Parallel Ocean Program (POP) and Sea Ice (CICE) models, which it originally developed and supplied to the project. Through the DOE Climate Change Prediction Program, SciDAC supplements work in Los Alamos's core funding.

Los Alamos's efforts have resulted in accelerating the development of a new Arbitrary Lagrangian-Eulerian vertical coordinate scheme in the POP ocean model and have added a new remapping transport scheme to the CICE model. The Laboratory's involvement has also enabled the design and integration of ocean biogeochemistry into the POP model and has focused on software process improvements in adopting a more formal design and testing process for the development of ocean and sea ice models.

The Impact: The Best Possible Model for Climate Change Studies

Current SciDAC efforts will advance work on the CCSM while providing collaborators, such as Los Alamos, with the best possible coupled climate model for use in climate change studies. Future work will create capabilities for performing carbon cycle modeling and permit the simulation of the full carbon cycle in coupled climate models in the biogeochemistry-atmospheric chemistry portion of this project.



Geodesic Quasi-Lagrangian Climate Model

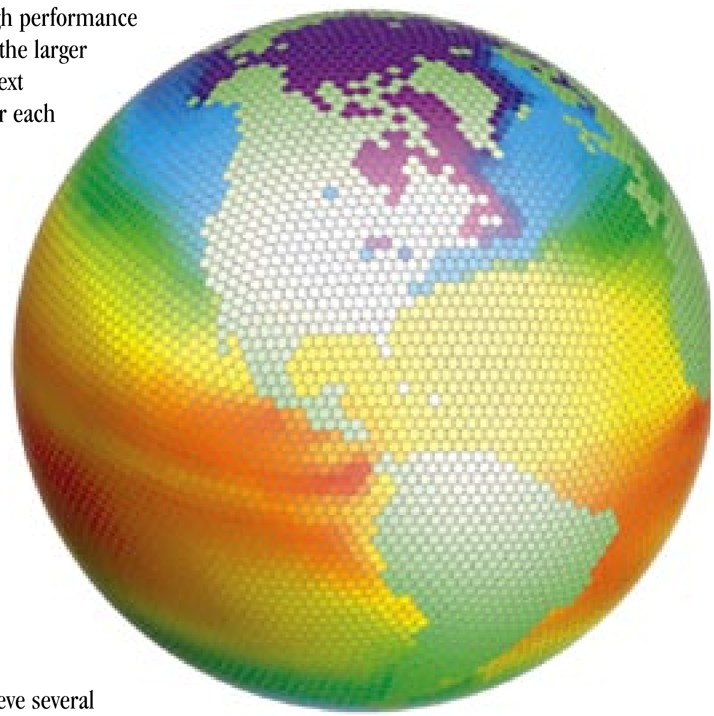
The Challenge: Predicting Climate Change on Long Time Scales

The Environmental Sciences Division of the Department of Energy has among its chief scientific objectives the development of a process to accurately predict climate change on decadal and longer time scales. The current phase of the DOE research effort is the Climate Change Prediction Program (CCPP). In support of the CCPP, Los Alamos is taking part in the Geodesic Quasi-Lagrangian Climate Model project. The project will develop a new model that is highly efficient for future high-performance computers as well as more accurate in its representation of physical reality and, therefore, will be more able to predict the future response of the climate system. This 5-year cooperative agreement is funded by the Scientific Discovery through Advanced Computing (SciDAC) program.

Los Alamos Innovation: Applying Existing Capabilities to a Geodesic Grid Model

Based on its demonstrated capabilities in developing ocean models for high performance computers, Los Alamos will provide the ocean and sea ice components of the larger coupled climate model. To the primary goal of this project—building a next generation global climate model using an almost uniform geodesic grid for each of the model's components—Los Alamos will contribute the following:

- Parallel Ocean Program (POP) code, which already serves as the ocean component in two of the nation's primary numerical climate models: the Community Climate System Model (CCSM) and the Parallel Climate Model (PCM);
- HYPOP model, which is a new hybrid vertical coordinate ocean model on a geodesic grid that has been developed over the past 2 years; and
- Geodesic grid models, which have provided the dynamical core algorithms for and assisted in the development of the new German Weather Service geodesic grid global weather forecast model and are currently in use in more than 20 countries.



An example of a geodesic grid with a color-coded plot distribution. The continents are depicted in white. This grid has 10,242 cells, each of which is about 240 km across. Twelve of the cells are pentagons; the rest are hexagons.

The Impact: Simplified Coupling of Models through a Universal Grid Geometry

With Laboratory contributions, the completed climate model will help relieve several computational difficulties by eliminating the polar singularities inherent in traditional latitude-longitude grids and simplify coupling of component models with a universal grid geometry for all models. The model will also allow for approximate Lagrangian treatment of vertical flow with hybrid vertical coordinates, except in the boundary layers at the Earth's surface, and provide higher computational efficiency on future generations of parallel supercomputers. It will also enable higher fidelity treatments of the atmosphere, ocean, sea ice, and land surface systems.

Los Alamos NATIONAL LABORATORY

Earth System Modeling Framework

The Challenge: Developing Flexible Software Tools for Earth System Modeling

The need for further development of flexible software tools for use in Earth system modeling has become increasingly apparent in recent years. To address the issue of excessive time and resources being expended on this challenge, the NASA Earth Science Technology Office (ESTO) funded the Earth System Modeling Framework (ESMF) collaboration. This 3-year effort involves Earth scientists and computational experts from Los Alamos National Laboratory and nearly all of the other major modeling centers in the climate and weather forecast communities. The ESMF collaboration is developing a robust, flexible set of software tools that will respond to the computational needs of increasingly complex models and platforms.

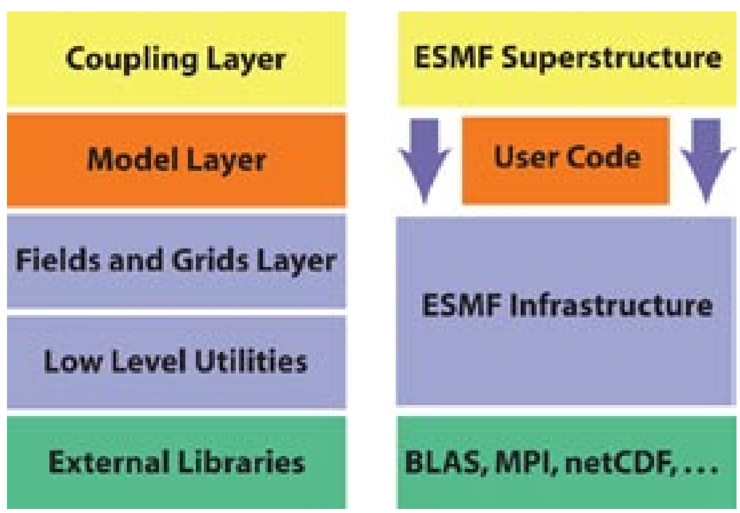
Los Alamos Innovation: Remapping and Regridding to Couple Models

As the developers of the Spherical Coordinate Remapping and Interpolation Package (SCRIP), Los Alamos will provide the ESMF with expertise in remapping and regridding functionality, which is critical for coupling together models on different grids. The Laboratory will implement the framework in the Parallel Ocean Program (POP) and Sea Ice (CICE) models to ensure these codes can interoperate with other component models in the framework.

To address these complex challenges and goals, Los Alamos is

- Implementing a redesign of the SCRIP software to meet the requirements of the ESMF and continuing to improve its capabilities and flexibility with testing of additional ESMF components; and
- Incorporating framework elements into the POP and CICE models as they become available to ensure the models are compliant with the ESMF.

The Impact: A Common Software Framework for a Diverse Community of Users



This diverse collaboration of proven expertise will ensure a framework will be implemented across a broad range of institutions to address the complex needs of the entire community. In addition, the development of a software interface specification will allow groups at all participating institutions and in all disciplines to generate interoperable software components. The result will be enhanced and improved data communication, model component coupling and sequencing, time management, and parameter specification.

The ESMF effort creates opportunities for Los Alamos-developed component models to be adopted by other modeling efforts. The Laboratory achieves greater flexibility in its response to new initiatives or global change issues, and its ability to incorporate new aspects of the climate system, currently not included in coupled models, is enhanced. Finally, ESMF permits Los Alamos to interoperate with other components and collaborate with a wider community to customize applications with the best components.

NASA Computation Technologies Project:
Applying the Earth System Modeling Framework to the El Niño-Southern Oscillation

The Challenge: Understanding the Global Climate Effects of the El Niño-Southern Oscillation

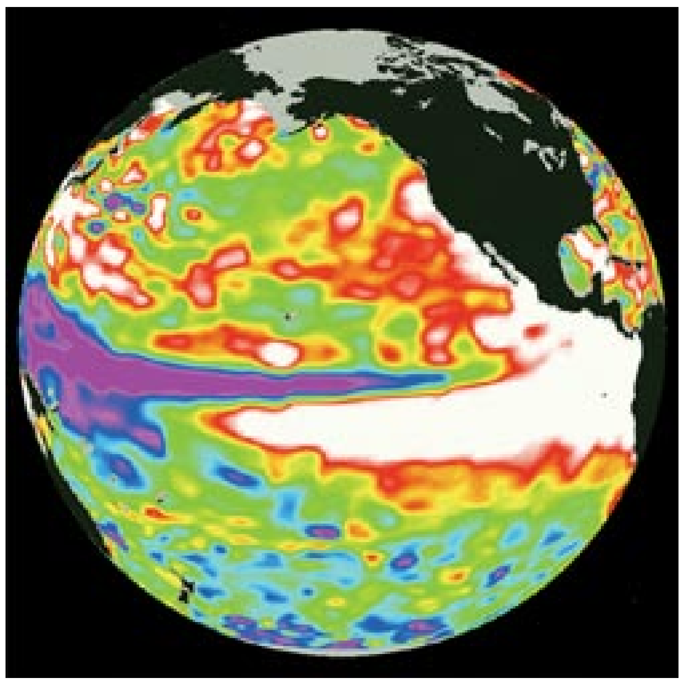
Developing an Earth System Modeling Framework (ESMF) is the focus of three of the current cooperative agreements of the Computational Technologies (CT) Project in the NASA Earth Science Technology Office. As part of a separate CT cooperative agreement headed by the University of California, Los Angeles (UCLA), Los Alamos will be using ESMF to couple its HYPOP ocean and CICE sea ice model with the UCLA atmospheric general circulation model as an early validation of ESMF functionality and efficiency. This undertaking will enhance coupled model simulations of the El Niño-Southern Oscillation and its global effects on climate.

Los Alamos Innovation: Seamless Coupling of Model Components

Based on its demonstrated capabilities in developing ocean and sea ice models for high-performance computers, Los Alamos was asked to provide the ocean and sea ice components of the larger coupled climate model. The Laboratory responded by developing a new hybrid vertical coordinate ocean model, known as HYPOP. This model provides an ideal opportunity for demonstrating ESMF ability to interchange model components in a largely seamless manner. Interpretation of vast quantities of observational data will be enhanced while the process of swapping and comparing alternative scientific approaches from varying research groups to improve the models' fidelity and predictive capabilities will be simplified.

The Impact: Realistic Simulations of Natural Phenomena

Los Alamos will now engage in an important university collaboration and a key NASA initiative to develop a software infrastructure for the climate modeling community. With Laboratory contributions, the ESMF will provide more realistic simulations of natural phenomena and eliminate time-consuming reprogramming by handling all communications in coupled climate models and enabling them to run on a variety of supercomputer architectures.



From measurements made by the U.S./French TOPEX/Poseidon satellite, this Pacific Ocean image shows sea surface height relative to normal conditions. The volume of warm surface water (white) represents the core of 1997/98's El Niño in the eastern Pacific Ocean. Green indicates normal; purple indicates cool.

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National Ocean Partnership Program (NOPP) Paradigm Project

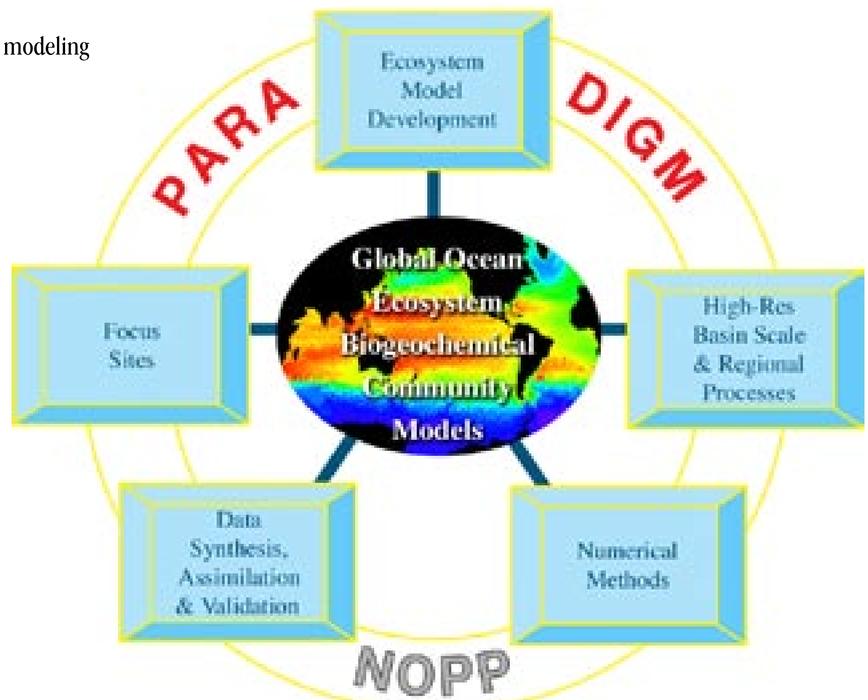
The Challenge: Including Marine Ecosystems in the Global Carbon Cycle Model

Modeling the full Earth system—which includes the ocean, sea ice, atmosphere, and biosphere—is an extremely complicated challenge that has not yet been met. An accurate model of the global carbon cycle must include marine ecosystems and other geochemical processes that naturally occur in the global climate system. Such a model would provide a greater understanding of ocean biogeochemistry to facilitate global change prediction. To address this issue, the National Ocean Partnership Program (NOPP) has sought the help of Los Alamos and 14 other institutions in order to implement the PARADIGM project.

Los Alamos Innovation: Advanced Biogeochemical Modeling

Los Alamos has accepted the challenge of providing the key research component for the community ocean circulation model and providing support for the development of the Parallel Ocean Program (POP) of the PARADIGM project. The Laboratory is employing its unique capabilities in high-performance computing and modeling and simulation to perform high-resolution ocean simulations with an imbedded ecosystem model for POP. This complicated ecosystem model describes the growth, decay, transfer, and evolution of almost 20 different species, ranging from 3 types of phytoplankton to dimethyl sulfide to carbon dioxide.

Used by other members of PARADIGM, the biogeochemical modeling performed by Los Alamos will result in the development of the next generation of ecosystem models and improve understanding of the carbon cycle while advancing knowledge of the environmental effects of greenhouse gases.



The Impact: A Fully Coupled Earth System Model

As a component of the Coupled Climate System Model (CCSM) at the National Center for Atmospheric Research, POP will be used in the future for fully coupled carbon cycle simulations which will further our understanding of global change. Los Alamos's contributions to POP have provided a valuable resource for carbon cycle research and global change prediction. The Lab's biogeochemical component of the POP project will bring the scientific community one step closer to a fully coupled Earth system model.

Tropical Climate Monitoring

The Challenge: Monitoring Global Climate

The Department of Energy's Atmospheric Radiation Measurement (ARM) Program has selected Los Alamos National Laboratory to manage its climate monitoring stations in the Tropical Western Pacific (TWP). Climate monitoring in the TWP is important for the following reasons:

- The TWP consistently has the warmest sea surface temperatures on the planet and is referred to as the Pacific "warm pool";
- The warm pool supplies heat and moisture to the atmosphere above it, resulting in the formation of deep convective cloud systems which, in turn, produce high altitude cirrus clouds that spread out over much of the region;
- These cloud systems regulate the amount of solar energy reaching the surface of the earth and the amount of the earth's heat energy that can escape to space.

Los Alamos National Laboratory recently began to manage the deployment, maintenance, and calibration of a new ARM Mobile Facility. The purpose of the mobile facility is to extend climate monitoring to regions of the globe that are not well characterized by the stations ARM presently maintains in the TWP, the Southern Great Plains, and the North Slope of Alaska.

Los Alamos Innovation: Managing Climate Monitoring Stations

The sites in the TWP locale include the islands of Nauru and Manus, Papua New Guinea, and a new facility built last year in Darwin, Australia. In addition to instrument calibration/maintenance and data quality assurance for ARM sites, Los Alamos's responsibilities include

- Foreign contract management,
- Local observer and visitor safety awareness,
- Site security,
- Power and communications (which can be undependable),
- Intermittent transportation, shipping, and import customs,
- Local government policies, and
- Cultural sensitivities and land ownership issues.

Atmospheric Radiation Measurement (ARM) sites—established stations in yellow and possible locations for the ARM mobile facility in blue.

The Impact: Producing High Quality and Continuous Data

The operation of the sites in the TWP region and the new mobile facility is designed to address the core mission of the ARM Program which is to

- Improve the performance of General Circulation Models (GCM's) used for climate research and prediction by improving the treatment of radiation transfer under clear sky, overcast, and broken cloud conditions; and
- Improve the parameterization of the properties and life cycle of clouds in the GCM's.

Los Alamos National Laboratory will maintain the infrastructure required to produce high quality and continuous data from a variety of sensors. These sensors range from *in situ* point measurements, through balloon-borne profiles, to complex remote sensing active and passive instrumentation. The data at the sites are also used to study important climate related phenomena such as the Southern Oscillation and as ground truth for satellite observations. The satellite observations range from continuous geostationary satellites, through relatively standard orbiting satellites such as AVHRR and MODIS, to special satellites such as the DOE Multispectral Thermal Imaging (MTI) satellite.

Resolving the Aerosol-Climate-Water Problem by Integrating Observations and Models

The Challenge: Predicting the Effects of Aerosols on Health, Climate, and Water

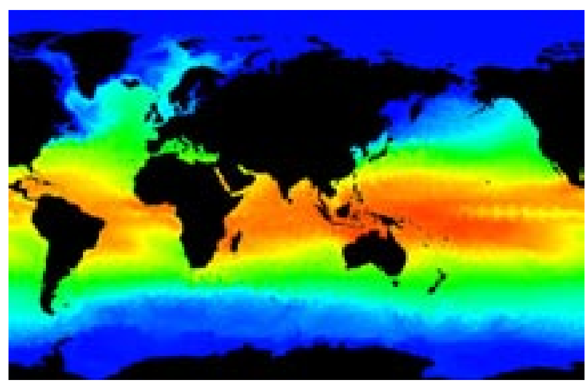
A pressing question confronting society is how particle emissions from human activity affect our health, global climate, and water supplies. The current scientific assessment of this aerosol problem faces some fundamental challenges:

1. Aerosol effects on climate are the most uncertain element in climate assessment. The problem is so severe that we do not know whether net effects of anthropogenic emissions (greenhouse gases and aerosols) are warming or cooling our climate.
2. Aerosols have been implicated in suppressed rainfall, persistent monsoon failures, and prolonged drought. If confirmed, such perturbations of the Earth's hydrological cycle could outweigh present concerns about global warming.

Quantifying the role of aerosols poses a scientific challenge because of their complex composition, range of lifetimes, ability to absorb and/or scatter solar and terrestrial radiation, and effect on cloud properties.

Above: Department of Energy's MultiThermal Imager (MTI) is used to examine clouds, aerosols, water, and surface properties.

Below: Simulated ocean temperatures in a Los Alamos ocean model.



Los Alamos Innovation: Linking Satellite Observations and Laboratory Experiments

Los Alamos is poised to tackle the aerosol problem with an integrated approach that couples observations, models, and experiments to capture processes and assimilate data in coupled-climate and atmospheric-transport models. We are linking three pillar capabilities at Los Alamos—remote sensing science, ocean-atmosphere modeling, and laboratory aerosol diagnostics—and collaborating with key external institutions (NASA, NCAR, and Scripps) to quantify the role of aerosols in climate change and to develop predictive tools to assess their long-range transport and impact on water resources.

The Impact: Rapid Aerosol Forecasting Tools

Los Alamos's efforts will provide predictive assessments of the impacts of aerosols on climate and water resources and will enable the development of next generation data assimilation methods for rapid aerosol forecasting tools.

Regional Climate Modeling

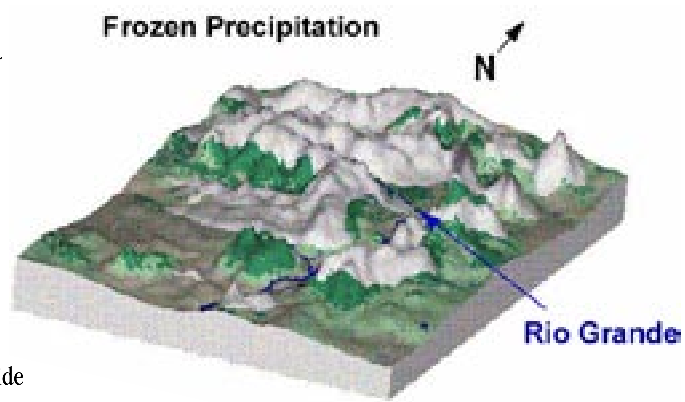
The Challenge: Predicting Climate Change Effects on a Regional Scale

The headwaters of the Rio Grande are located in the San Juan Mountains of southwestern Colorado and the upper portions of the river are fed primarily by snowmelt from winter storms. In contrast, the lower portions of the river accumulate runoff from thunderstorms of the summer monsoon season. Consequently, the waters of the Rio Grande are strongly influenced by regional climate and could be vulnerable to climate change. Since precipitation and runoff in arid regions are low and highly variable, improved knowledge of the climate and hydrology is essential for optimal management of water resources in the Rio Grande basin and other arid regions of the world. It is important to understand the entire hydrologic cycle and to be able to explore the potential effects of increased water use and of changes in global and regional climate. Global climate models (GCMs) utilize grids that are too coarse to resolve changes in regional climate and the predictions for a particular region vary depending on which global model is used. Therefore, the results of global climate predictions need to be downscaled to extrapolate the global predictions to regional relevance. Regional climate models can dynamically downscale global climate predictions to a more usable resolution.

Los Alamos Innovation: An Interactive System of Atmosphere, Surface, and Groundwater Models

The research reported here is part of a larger project that is coupling a suite of environmental models to simulate the hydrologic cycle within river basins. These models include the Regional Atmospheric Modeling System (RAMS) which provides meteorological variables and precipitation to land surface hydrology models. To downscale global climate predictions, RAMS can use GCM-predicted meteorological fields to initialize and nudge the model fields. The surface hydrology model partitions the precipitation into evaporation, transpiration, soil water storage, surface runoff, and subsurface recharge. The surface hydrology component is being updated to include the TIN-based Real-time Integrated Basin Simulator (tRIBS), developed at the Massachusetts Institute of Technology (MIT). The runoff is collected within a simple river channel model and the Finite Element Heat and Mass (FEHM) subsurface model is linked to the land surface and river flow model components to simulate saturated and unsaturated flow and changes in aquifer levels. Our goal is to produce a fully interactive system of atmospheric, surface hydrology, river, and groundwater models to allow water and energy feedbacks throughout the system.

Spatial distribution of frozen precipitation (white) over the RAMS third grid, which includes the upper Rio Grande Basin to Albuquerque, NM. The green shades represent the topography, from lighter shades at lower elevations to darker shades at higher elevations.



The Impact: Evaluating Changes in Regional Extremes

This approach will allow us to examine changes in regional extremes for properties such as precipitation and temperature that cannot be obtained from global climate model simulations because of their coarse resolution. Los Alamos's regional climate simulations can provide planning tools for water resource managers and planners in regions of concern.

Distributed Hydrological System for Modeling Water Resources

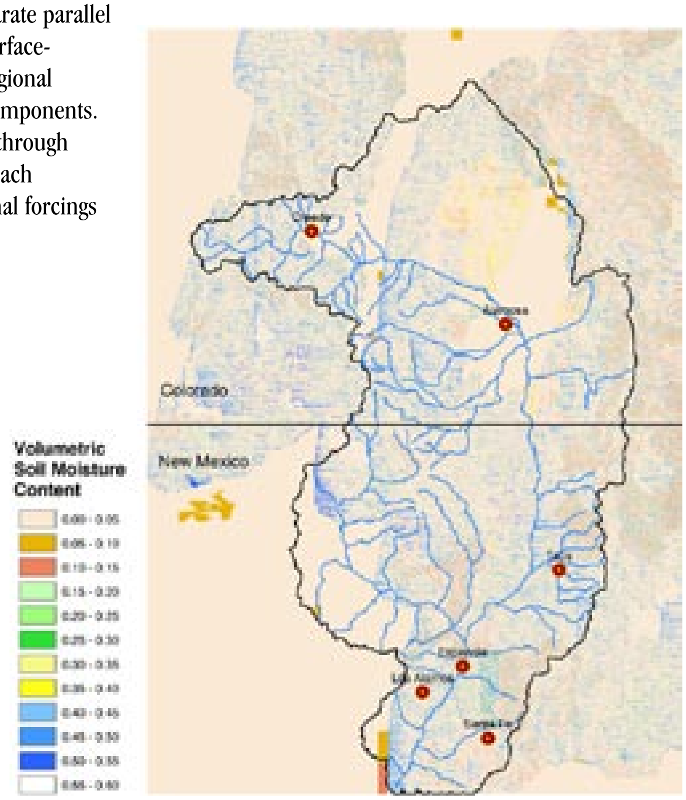
The Challenge: Meeting Increasing Demands for Water Resources

With limited supplies and increasing demands for water resources, especially in arid and semi-arid regions, it is becoming increasingly important to understand the workings of the hydrologic cycle within river basins. A thorough understanding of typical precipitation, runoff, and groundwater and the nature of the their variability is vital for planning the best use of these water resources. In the long term, all aspects of the hydrologic cycle affect the availability of water and it is therefore important to explore the entire cycle in order to understand the potential effects of increased water use and of changes in the regional climate. Allocations of scarce natural resources like water can be based on detailed computational models of complex natural-human systems.

Los Alamos Innovation: Coupling Existing Models to Form a Single Virtual Watershed Model

To simulate water resources, Los Alamos researchers are coupling a series of existing and previously tested models in a single virtual watershed model that addresses the multitude of physical processes and temporal and spatial scales that are important. The Los Alamos Distributed Hydrologic System (LADHS) currently emphasizes natural processes, but components can be extended to include such anthropogenic processes as municipal, industrial, and agricultural demands. LADHS is composed of four interacting components: a regional atmospheric model, a land surface hydrology model, a subsurface hydrology model, and a river routing model. The system is embedded in the Parallel Applications Workspace, which is a software infrastructure for connecting separate parallel applications within a multi-component model. Integrated atmosphere-land surface-groundwater models like LADHS provide a more realistic assessment of the regional water balance than separate models can by including feedback between the components. For example, boundary conditions from global climate models can propagate through the virtual watershed and the effects of interactions can then be evaluated in each component. Many of these components are nonlinear and the effects of external forcings are not readily predictable.

Soil moisture field—the black outline depicts the boundaries of the upper Rio Grande basin.



The Impact: Effective Management of Water Resources

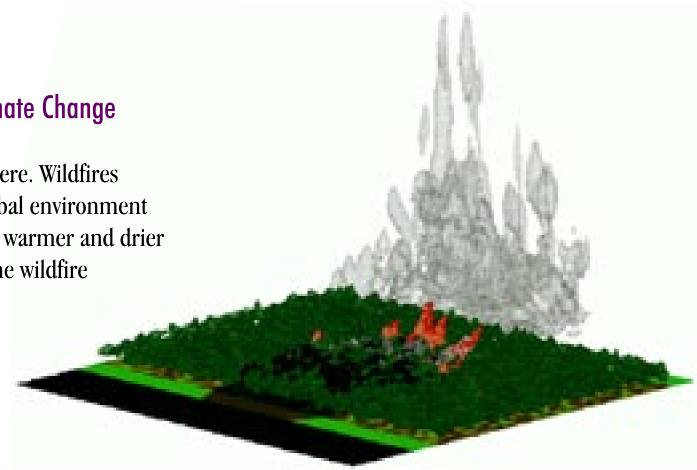
Los Alamos's virtual watershed model, the Los Alamos Distributed Hydrologic System, retains the essential physics of all elements of a regional hydrosphere and allows feedback between them. At the highest level of description, LADHS functionality reflects exchanges of mass and energy between physical elements of the regional hydrosphere. Results of initial simulations of the water balance between the land surface and atmosphere in the upper Rio Grande basin illustrate the promise of this approach. Compared to real watersheds, virtual watersheds are cheap to produce and allow experimentation. They are flexible enough to accommodate novel boundary conditions like land use change and increased climate variability. Decision-makers can use virtual watersheds to evaluate the risks of management alternatives once uncertainties have been quantified.

Los Alamos NATIONAL LABORATORY

Climate Change and Wildfire Emissions

The Challenge: Understanding the Effects of Wildfire Emissions on Climate Change

Wildfire emissions are a major source of carbon and aerosols in the atmosphere. Wildfires are local to regional scale phenomena that have the potential to affect the global environment through atmospheric transport processes. Climate change scenarios describe warmer and drier environments in various areas around the globe that can lead to more extreme wildfire behavior and their associated emissions. At present, the impact of evolving environmental conditions on fire emissions is highly uncertain, due to a lack of data and simulation tools that can adequately describe complex fire behavior and chemistry.



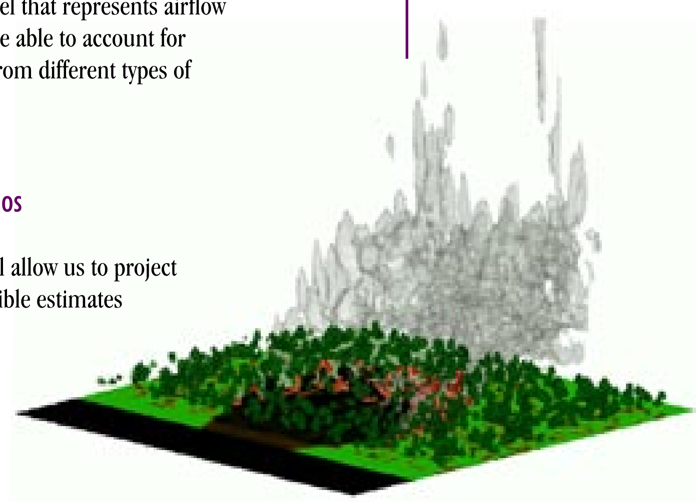
Los Alamos Innovation: A Physics-Based Wildfire Model

Over the past eight years, Los Alamos has developed a unique physics-based fire behavior model, HIGRAD/FIRETEC, that can begin to provide answers to fire emissions questions for better understanding of global climate change problems. HIGRAD/FIRETEC is the first physics-based, three-dimensional (3-D) computer code designed to simulate the constantly changing, interactive relationship between fire and its environment. It does so by representing the coupled interaction between fire, fuels, atmosphere, and topography on a landscape scale (hundreds or thousands of meters). HIGRAD/FIRETEC combines physics models that represent combustion, heat transfer, aerodynamic drag, and turbulence with a computational fluid-dynamics model that represents airflow and its adjustments to terrain and vegetation structure. The model will also be able to account for differences in the combustion, aerosol production, and emissions resulting from different types of fuels.

Wildfire simulation with FIRETEC in a dense (above) and less dense (below) forest stand showing flame intensity (red) and fire emissions (gray).

The Impact: Credible Estimates of Wildfires for Climate Change Scenarios

With some additional modifications, the HIGRAD/FIRETEC modeling suite will allow us to project greenhouse gases from wildfires of various fuel types and begin to make credible estimates of total greenhouse gas emissions from wildfires in climate change scenarios, taking into account statistically projected changes in numbers of wildfires worldwide due to changing temperature, moisture, and ecosystem health.



Climate Change and Ecosystem Dynamics

The Challenge: Understanding the Complex link Between Climate Change and Vegetation and Ecosystem Dynamics

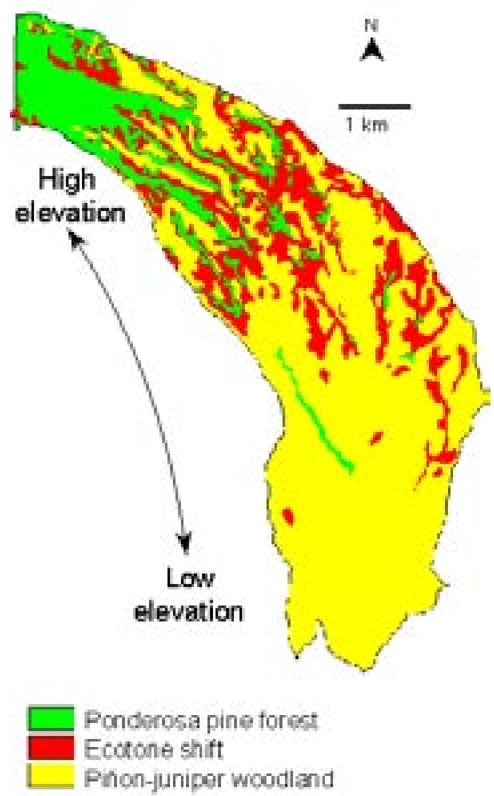
Climate is a key driver of vegetation dynamics and associated ecosystem changes. Changes in vegetation and ecosystem processes can also have important effects on climate and weather patterns. This interrelationship between climate and vegetation pattern/ecosystem properties is particularly pronounced in dryland environments, where water is so intimately tied to energy and carbon budgets. Researchers at Los Alamos National Laboratory are focusing on how water, energy, and carbon are affected and/or affect vegetation patterns and dynamics.

Los Alamos Innovation: Increasing Understanding of Ecosystem Processes

Studies of piñon-juniper woodlands and ponderosa pine forests at Los Alamos have significantly increased our understanding of ecosystems processes. Results of these studies include the following:

1. Quantification of the most rapid landscape scale response of an ecotone (a boundary between two ecosystems) documented to date in response to climate. During the 1950's drought, the ponderosa pine forest/piñon-juniper woodland ecotone shifted more than 2 km in less than 5 years. These results have important implications for assessments of ecosystem responses to climate variability and change.
2. Quantification in a piñon-juniper woodland of spatial heterogeneity in near-ground solar radiation, soil temperature, soil water content, snow cover, runoff, and erosion. This is the most intensely instrumented piñon-juniper woodland plot in existence.
3. Development of a model for transitions from low rates of runoff and erosion to high rates of runoff and erosion.
4. Development of a conceptual model relating both horizontal and vertical heterogeneity in soil moisture to plant community composition and dynamic responses to climate and land use.
5. Demonstration that interflow (shallow subsurface flow) in a semiarid ponderosa pine forest is a substantial part of the water budget. This is the first demonstration of the importance of this process in a semiarid environment.
6. Development of a spatially explicit ray-tracing model of solar radiation that has been used to quantify general trends in the spatial distribution of solar radiation as a function of changes in the proportions and patterns of woody plants.

Tree stand changes In Bandelier National Monument, New Mexico during the 1950's drought.



The Impact: Predicting the Interrelationships Between Climate and Vegetation

Los Alamos National Laboratory's data sets and modeling capabilities in ecology provide critical assets necessary to address emerging climate problems. In particular, through extensive field research we have developed many unique data sets and models that are central to evaluating the predictive interrelationships between climate and vegetation.

Paleoclimate Records and Climate Change in the Southwest

The Challenge: Examining Past Climate Cycles to Predict Future Water Availability

Understanding climate cycles that control the hydrologic cycle is the key to predicting future water availability. While instrumental records of climate and weather patterns only extend back approximately 100 years, proxy records of climate for hundreds of thousands of years can be reconstructed from tree rings, corals, ice cores, peat bogs, and speleotherms. Los Alamos is taking part in a pilot project funded by the University of California Institute of Geophysics and Planetary Physics to examine climate records contained in peat bogs from sites in the Jemez Mountains of North Central New Mexico.

Los Alamos Innovation: Applying Isotopic Expertise to Study the Environmental Record

The project will draw upon Laboratory capabilities in water and carbon research as it builds on previous work by Northern Arizona University, where research expertise in traditional paleo-environmental techniques has revealed significant climate variability in the semi-arid southwest. The state-of-the-art facilities and history in isotopic studies at Los Alamos provide technical expertise in light stable isotope environmental reconstruction and dating techniques that include both optically stimulated luminescence and uranium-series dating.

The Impact: Predicting the Occurrence and Magnitude of Future Droughts

With future climate change affecting water availability for agriculture and energy production as well as for industrial and household use, this study will focus on reconstructing a 10,000 year record of climate/drought variability in mountainous regions of the semi-arid southwest that can then be analyzed for underlying periodicities. The study will also help to determine if anthropogenic effects have changed the periodicities of phenomena such as the Pacific Decadal Oscillation, which results in long-term drought in the southwest. Ultimately, this work will provide climate time series that will be analyzed in terms of drought frequency, allowing prediction of future drought timing and magnitude. This work will also form the basis of future Los Alamos efforts to couple observational/experimental science with global change modeling efforts to address national issues of energy security, water security, wildfire risk, and environmental sustainability.

Ancient lake sediments in the Valles Caldera.

Warming Trends and Water Resources

The Challenge: Adapting to Rising Temperatures and Resulting Hydrological Changes

Warming trends have become apparent in the last forty years and are expected to accelerate in the 21st century. Current models also predict evaporation of more water vapor into the lower atmosphere. In regions with most of the world's population, societies will probably have to adapt not only to significant temperature rises, but also to profound hydrologic changes and increasingly intense and frequent convective storms. These storms cause most flash floods and all large hail, microburst winds, lightning, and tornadoes. In addition to generating severe weather, convective storms play two key roles in the climate system. First, they are the principal vertical transport path for water and latent heat between the lower and upper troposphere. This is key to the Walker and Hadley cells of low-latitude heat transport. Second, robust convective storms that overshoot the tropopause ("penetrative convection") inject cloud ice into the normally dessicated stratosphere. Stratospheric ice alters the radiative balance (via the visible albedo) and also serves as a host substrate for trace-gas heterogeneous chemistry (e.g., the sink for stratospheric ozone).

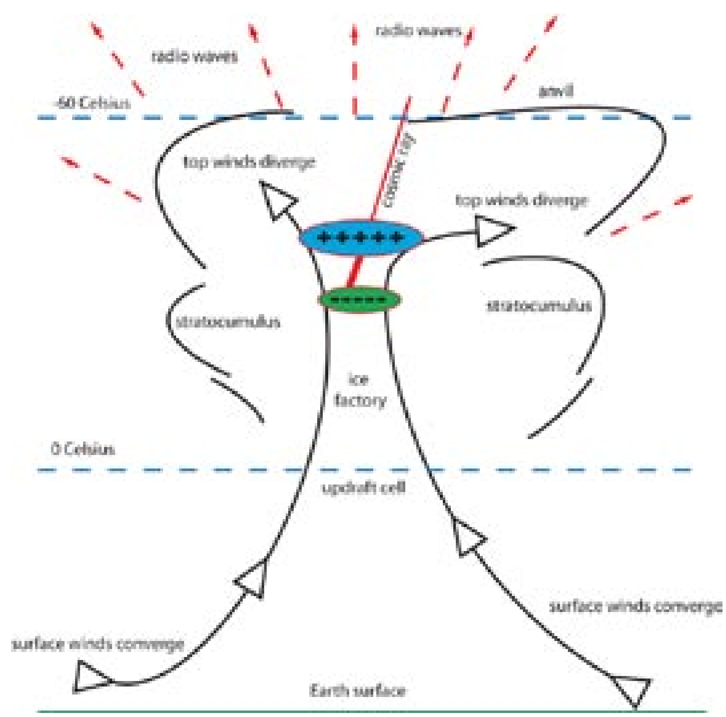
Los Alamos Innovation: Locating and Characterizing Storms by Analyzing Their Radio Emissions

During the 1970's, NASA Goddard scientists discovered spectacular radio emissions from convective storms. These radio emissions were approximately 100 times more intense than those ordinarily associated with lightning. Later, in the 90's, Los Alamos National Laboratory participated in the development of satellite platforms, ALEXIS and FORTE, which showed that these radio signals were the most likely weather-associated radio signals to be observable from space. The FORTE satellite, launched in 1997, performed simultaneous radio and optical observations of lightning and demonstrated that the pulses are unassociated with detectable luminous signals; that is, the intense radio pulses are "dark lightning." Moreover, the radio pulses are not the signatures of conventional electrical breakdown of the air, although such breakdown can be instigated by whatever causes the pulse. Indeed, conventional breakdown is sometimes observed to occur after one of the bright pulses is emitted. Detection of these radio pulses from storms indicates the location and severity of significant tropospheric convection. Detection can be done from the GPS constellation by instruments that Los Alamos National Laboratory designs, builds, and maintains.

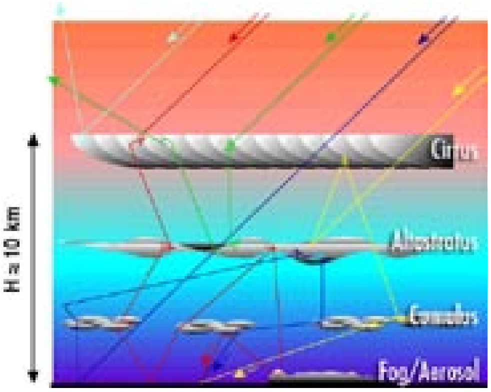
The Impact: Environmental Security

The U.S. government is aggressively emphasizing a national strategy of adaptation to climate change. Significant new support is planned for an adaptive (as opposed to a preventive) national climate program. Los Alamos National Laboratory's capabilities are perfectly aligned with this strategy of adaptation which aims to employ sophisticated sensor networks to provide timely and accurate warning of developing outbreaks of severe weather that have the potential to harm people, communities, aviation, and facilities. To succeed, the nation urgently needs scientific and technical breakthroughs in detection and tracking of nascent, severe, convective storms, globally and in real time.

An intense updraft generates layers of positive and negative charge high in the updraft cell. Incident cosmic ray (solid red line) instigates relativistic-avalanche breakdown (heavy line) in region of high electric field between charge layers. Radio-wave emissions provide means for real-time satellite retrieval of 3-D position of breakdown. Between the 0 and -60 Celsius isotherms is the region of mixed-phase hydrometeors (graupel, ice crystals, supercooled droplets). This mixed-phase condition requires a sustained and intense (>15 m/s) updraft with copious water entering (as vapor) from the ground-level convergence. The updraft-core diameter is a few kilometers.



Cloud-Radiation Interactions in Climate Modeling and Remote Sensing



Above: Cloud opacity forces light to bounce randomly. Tenuous regions inside clouds, gaps between clouds and cloud layers enable very large jumps, making the diffusion process “anomalous.” Statistics for the total length of the convoluted photon paths from top-of-atmosphere to ground support the anomalous diffusion model.

The Challenge: Reduce Uncertainty from Clouds in Global and Regional Climate Models

Clouds are one of the most poorly understood parts of the climate system even though their impact on global heating and cooling is far stronger than aerosols, and as great as, if not greater than, all anthropogenically created or boosted greenhouse gases. Only water vapor surpasses clouds, which are just liquid or ice water particles small enough to not precipitate but large enough to scatter and absorb sunlight and thermal radiation. To complicate the issue, man-made aerosols (e.g., pollution, biomass burning) can modify cloud optical properties for scattering (reflection back to space) and absorption (atmospheric heating and re-emission). Anthropogenic particulates can also alter cloud life cycles, including the suppression of rain in some regions.

Los Alamos Innovation: Breaking Away from the Conventional "Slab-Cloud" Model

Clouds can be investigated from below (using radiometers and/or lasers), from within (primarily using aircraft), or from above (especially using space assets with imaging capability). They are so variable in space and time that there is never enough data, especially of the *in-situ* kind that we trust the most. Satellite remote sensing brings the greatest expectations. However, the algorithms used to infer cloud properties from observed radiances as well as the energy balance computations for climate modeling depend on radiative transfer theory. In essentially all such operational settings, this theory is predicated on the unrealistic assumption that clouds are infinite, uniform slabs because that geometry is historically perceived as the only tractable case. At Los Alamos, we have developed new radiative transfer models targeting either the radiative energy budget or remote cloud diagnostics that account for the 3-D variability of clouds. Our innovative observation methods are both passive (sunlight-based) or active (laser-based) as in the case of Wide-Angle Imaging Lidar. The new radiative energy partition models are by design amenable to the contrasting situations where we know either very little or a lot about 3-D cloud variability, all depending on the scales of interest.

Below: Broken clouds (from DOE’s high-resolution Multispectral Thermal Imager satellite) not amenable to the standard “slab” model used in remote sensing. Our finite-cloud algorithm uses reflected and transmitted radiance and gives good results for the three indicated cases with different sizes.

The Impact: Eliminating Biases in Cloud and Climate Dynamics, Renewing Cloud Remote Sensing

The hallmark of cloud radiative transfer modeling at Los Alamos is to go beyond the use of 3-D theory to quantify the error in standard methodology, which typically ignores all cloud variability inside a satellite’s cloudy pixels or inside a climate model’s grid cells. We propose effective mitigation strategies. For instance, we have developed

- 3-D remote sensing methods specifically for broken or isolated clouds (see lower figure);
- “Off-beam” lidar systems that can penetrate opaque clouds using scattered laser photons;
- An efficient physics-based method for estimating heating and cooling at every point inside a 3-D cloud as it is dynamically modeled;
- An anomalous diffusion model for the mean radiative fluxes through the whole atmospheric column (see upper figure).

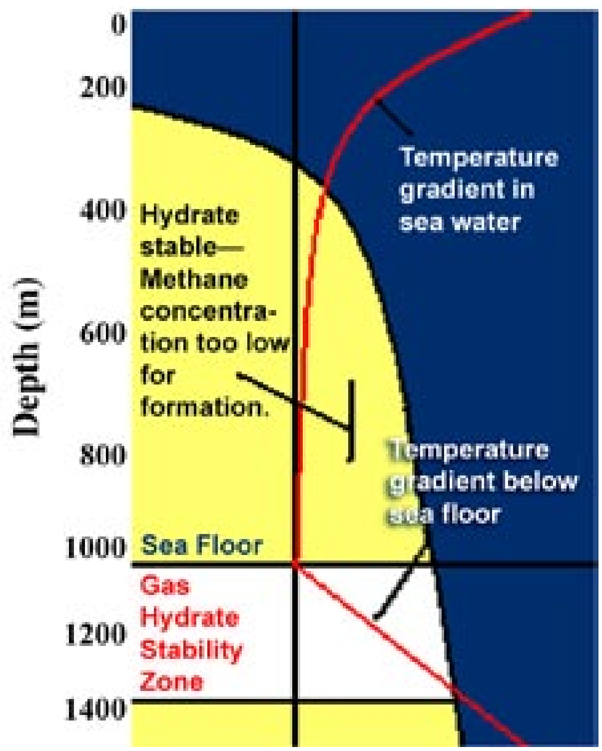
This last model has successfully explained the variability of new photon path length observations using oxygen-line spectroscopy at very high resolution.

Producing Fuel and Managing Waste with Oceanic Gas Hydrates

The Challenge: Developing New, Non-Polluting Energy Resources

The countries of the world currently burn the equivalent of 60 billion barrels of fossil fuel per year, emitting seven billion tons of carbon in the form of CO_2 into the atmosphere. The atmospheric CO_2 concentration has increased from 280 ppmv (parts per million by volume) in the year 1800 to 370 ppmv in 2000. This increase is closely linked to global climate change. Energy consumption and CO_2 emissions continue to increase each year. As the largest energy consumer in the world, the United States relies on fossil fuel imports to make up its 20% shortage in energy production. Such reliance on foreign resources is not conducive to national energy security. These two issues—climate change and reduced reliance on foreign energy sources—will most likely dominate future energy planning.

Methane hydrate phase boundary (the half bell-shaped curve) and the sea water temperature profile (red line). Based on this temperature profile, it is possible to find methane hydrates on the sea floor at a 400 m depth. The methane concentration affects the actual depth where hydrates can be found (or mined).



Los Alamos Innovation: A Viable Strategy for Using Methane Hydrates

Over the last two decades, ocean exploration has uncovered a new fuel source—methane hydrates. Methane hydrates are usually found in ocean sediments on the sea floor of continental shelves or slopes (at a depth range of 350 m to 1200 m). The molecular structure is similar to ice except a methane molecule is trapped within the hexagon cage of ice. Methane hydrates exist in meta-stable equilibrium with their environment and are affected by changes in pressure and temperature. When it dissociates, due to either lowering pressure or rising temperature, the methane gas escapes and the ice cage melts. The chemical energy stored in methane hydrates is estimated to be twice that of all other fossil fuels combined. The technology to mine this new resource is not currently available, but Los Alamos is working on a viable strategy to use methane hydrates as a fuel source. The general proprietary design is a "closed system" (that is, no pollution byproducts will be emitted from the fuel cycle). While the concept requires additional refinement and investigation before being made available for marketing, the Laboratory anticipates looking for partners interested in engineering design studies in the near future.

The Impact: National Energy Independence and Reduced Greenhouse Gas Emissions

A methane hydrate closed energy cycle would reduce U.S. dependence on foreign energy supplies and help control the primary culprit in global warming—greenhouse gas emissions.

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Environmental Benefits and Risks of a Hydrogen Economy

The Challenge: Preparing for Risks Posed by Transition to a Hydrogen Economy

Hydrogen is likely to play a prominent role in delivering non-polluting energy to society. Hydrogen fuel cell technologies deliver high efficiency and their large-scale implementation promises to benefit human health by enhancing urban and regional air quality. Hydrogen could also reduce risks of climate change if its large-scale production by renewable or nuclear energy sources becomes viable. While it is well known that the byproduct of energy produced from hydrogen is water vapor, it is not well known that the storage and transfer of hydrogen is inevitably accompanied by measurable leakages of hydrogen. Unintended consequences of hydrogen leakage include a reduction in global oxidative capacity, and an increase in stratospheric water that could exacerbate halogen-induced ozone losses as well as impact the Earth's radiation budget and climate. An environmental risk-benefit analysis is clearly needed to guide policy for, and guide the development of, a hydrogen economy.

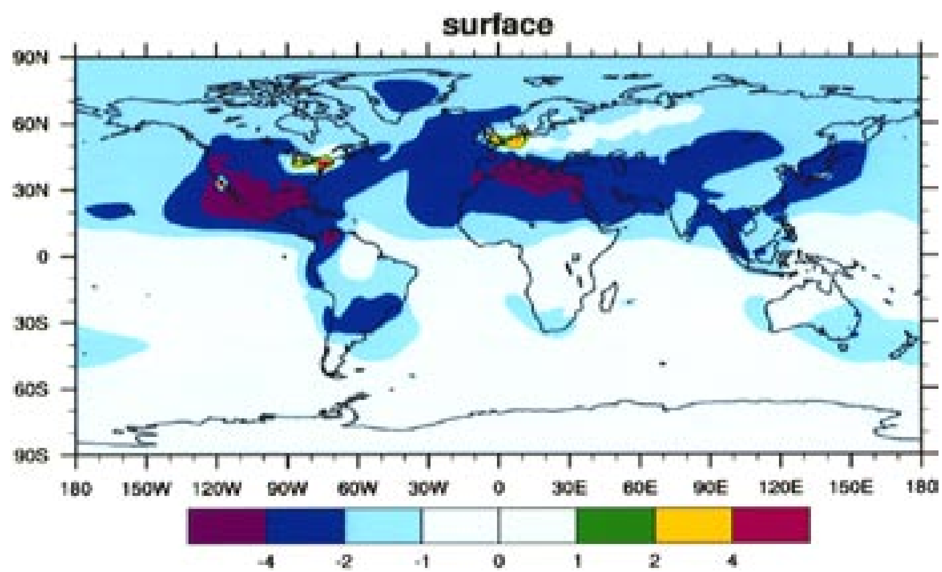
Los Alamos Innovation: Using a Global Atmospheric Model to Study Hydrogen Economy Scenarios

Los Alamos is using a global atmospheric model to examine the impacts of various hydrogen economy developments and leak scenarios on atmospheric chemistry. We are focusing on the effects of a reduction of nitrogen oxides from switching to fuel cells, as well as leaks from the production, distribution, and use of hydrogen. These include the improvement of air quality on a regional scale and a reduction of global oxidative capacity. We are also examining the increase in stratospheric water and its potential for increasing halocarbon-induced ozone levels there.

The Impact: Defining Tolerable Leak Rates for a Hydrogen Economy

Los Alamos's environmental risk-benefit analysis will define environmentally tolerable leak rates for a global hydrogen economy and provide a proactive approach to implementing new energy technologies in the 21st century.

Global model calculations of reductions in tropospheric ozone (smog) in parts per billion if we switch the power and transportation sector from fossil fuels to hydrogen thereby eliminating the emissions of nitrogen oxides and hydrocarbons.



New Approaches in Numerical Methods for Climate Modeling

The Challenge: Developing Accurate Numerical Climate Models

Numerical modeling is essential for understanding human impact on climate, but climate simulations intrinsically contain errors that could prevent accurate assessments. Contributing factors include imperfect knowledge of physical processes and numerical errors due to discretization of continuum equations. Even perfect models of physical processes can produce incorrect or misleading results when discretization errors are not controlled. Hence, it is important to understand and minimize the role discretization errors play. Climate simulations are routinely run for millions of time steps and thus significant build-up of time discretization errors can occur during a given simulation. Also, climate simulations typically employ very coarse spatial resolution and hence spatial discretization errors could be as large or larger than the temporal errors. Unfortunately, because current climate models do not monitor either type of discretization error, the impact of these errors on climate model predictions cannot be assessed.

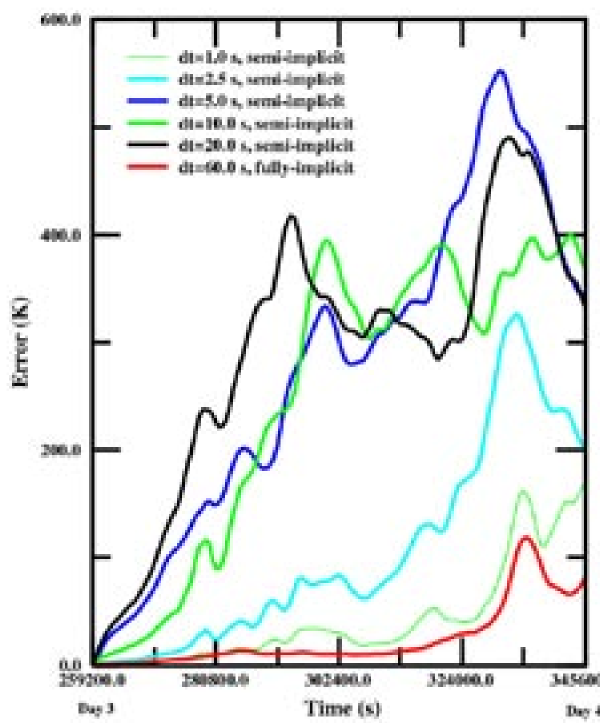
Another important source of error present in current climate models is that they all employ a time splitting or "divide and conquer" approach to solving their nonlinear physics packages. This approach can destroy natural force balances present in climate regimes. For example, by splitting fluid dynamics calculations from those related to cloud processes, large-scale balances produced by this interaction could be significantly altered.

Los Alamos Innovation: Combining Nonlinear Solution Procedures with Time Stepping Approaches

To quantify the magnitude of time splitting errors in climate simulations, new numerical frameworks must be developed. A numerical framework currently being tested involves the use of a nonlinear solution procedure, the Jacobian-Free Newton-Krylov approach (JFNK). When combined with higher-order Runge-Kutta time stepping approaches, the JFNK procedure is able to monitor both the evolution of temporal errors and to adapt the time step size to minimize their impact on a simulation.

The figure to the right shows a first attempt to quantify the time splitting error for a simulation relevant to atmospheric science, a three-dimensional idealized hurricane simulation. Even in this relatively simple problem run for a short time period, the temporal error growth in simulations employing decoupled physics packages is considerably larger than from a simulation employing a coupled physics package.

Another problem with traditional numerical approaches is that they do not converge the nonlinearities associated with the different physical processes, so these approaches can readily miss important time scales in the problem with the result that the accuracy of their forecasts is significantly degraded. The JFNK solution procedure can help determine whether time-scales in physics packages are being violated by lack of convergence of the nonlinear solver.



Errors in an idealized 3-D hurricane simulation, using decoupled and fully-coupled methods (JFNK approach). The fully-coupled method uses the largest time step but still has the smallest error. The error grows over time in all simulations.

HYDROGEN

Energy and Environment Compendium

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LALP-04-026

Hydrogen Research at Los Alamos National Laboratory

The Challenge: Clean Energy and Energy Independence

National and global energy needs are rising as the world population continues to grow and developing countries endeavor to offer their citizens a standard of living that equals that of more developed countries. Recent world events have increased public awareness of the energy, environmental, and security challenges caused by dependence on petroleum imports. To ensure safe, dependable energy supplies for the country and the world, more advanced resources must be developed to meet growing energy needs.

Hydrogen and Fuel Cells: The Promise and the Challenge

In its 2001 report, the National Energy Policy Development Group declared that hydrogen and other alternative energy technologies show great promise for providing the cleanest possible energy cycle. Hydrogen and fuel cell research have several challenges that must be addressed for innovation to continue in this field:

- **Better understanding of fuel cell system operation—** Conducting basic research to determine how fuel cells and supporting technologies work is the key to enabling knowledge-based innovation.
- **Data acquisition and experimental design—**Understanding and predicting phenomena in operating systems requires advanced diagnostic techniques to gather meaningful data from experiments.
- **Advanced modeling, simulation, and prediction—**Creating integrated models based on fundamental theory and acquired data is essential to understanding fuel cell issues, designing experiments within the model, and predicting fuel cell performance.
- **Proof-of-concept devices and systems—**Evaluating complex devices and systems requires multidisciplinary teams with access to diverse capabilities for innovative proof-of-concept demonstrations.
- **Knowledge and technology transfer—**For benefits in the areas of energy, environmental, and economic security, research and development must lead industry in developing fuel-flexible, efficient, clean, and affordable power systems for widespread use.

Los Alamos Capabilities in Hydrogen and Fuel Cell Research

In 1977, Los Alamos received Department of Energy funding to begin research into hydrogen as a renewable domestic energy carrier that would reduce emissions-based pollution and lessen the nation's dependence on foreign oil. Los Alamos has been building on this idea ever since.

Hydrogen and fuel cell research at Los Alamos has made significant technological advances in Polymer Electrolyte Membrane (PEM) fuel cells, Direct Methanol Fuel Cells (DMFC), and related technologies including the electrolyzer (a fuel cell in reverse, liberating hydrogen from electricity and pure water). With Los Alamos advances, these technologies may now be used in a variety of civilian power applications, including portable electronics, transportation, and combined heat and power for residential, commercial, and industrial buildings. To address the current scientific challenges faced by the hydrogen and fuel cell research community, Los Alamos has unique expertise and resources in

- **Electrochemical materials and devices—**The Laboratory has the leading expertise in developing fuel cell components (e.g., thin-film electrodes, membrane electrode assemblies, fuel cells, and electrolyzers).
- **Catalyst design, synthesis, characterization, and testing—** Los Alamos has the capability to design, synthesize, characterize, and test both electrocatalysts and catalysts for the various supporting systems.
- **Observational and experimental methods—**With sophisticated observational and experimental methods, the Laboratory can systematically capture fuel cell operation and degradation data.
- **Theory, modeling, and simulation—**Los Alamos has expertise in developing hydrogen- and fuel cell-related models at all scales, from molecular interactions to complete complex power systems.
- **Materials characterization and analytical chemistry—**The Laboratory's expertise in materials characterization and analytical chemistry is key to identifying and resolving fuel cell performance and degradation issues.
- **The Los Alamos knowledge base—**The Laboratory's databases, models, publications, and patent portfolio offer valuable resources to facilitate deeper understanding of phenomena and issues.

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- **High-performance computing—**The high-performance computing facilities at the Laboratory provide unparalleled speed that enables researchers to execute complex simulations.
- **Multidisciplinary approaches to complex systems—**Los Alamos approaches scientific and engineering challenges from several directions through expert multidisciplinary teams.

Hydrogen Fuel Cells for Power and Transportation

The Challenge: Less Dependence on Petroleum

Energy is consumed largely by three end-use sectors in the United States: buildings, industry, and transportation. Of the three, transportation consumes 27% of total U.S. energy and 67% of U.S. petroleum, and is 95% dependent on petroleum as an energy source. Given recent global events, diversifying the energy sources used to power vehicles has become a widely accepted goal.

Los Alamos Innovation: Hydrogen-Based Technologies

Recognizing these challenges nearly 30 years ago, Los Alamos began researching and developing means of using hydrogen as a petroleum alternative. In recent years, the Laboratory has developed demonstration hydrogen power systems. In hydrogen-powered transportation, Los Alamos has joined with General Motors (GM) to research methanol fuel processing and cleanup and liquid-fueled electrochemical engines. In the 1990's, Los Alamos and GM collaborated to create the Joint Development Center (JDC). Following the successes of the JDC, the Laboratory continued its own Fuel Cells for Transportation research program for the Department of Energy.


USCAR

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WHITE HOUSE HONORS AUTOMOTIVE RESEARCHERS

PNGV Medal Awarded for Breakthrough on Fuel Cells

Los Alamos National Laboratory researchers were honored for advances in fuel cell technology developed under the collaborative industry-government Partnership for a New Generation of Vehicles.

In addition to improving the power density, durability, and efficiency of energy conversion in fuel cells, current Los Alamos efforts are enabling distributed heat and power generation from diverse domestic resources. The project's tasks include

- Exploring ion-transport theory and modeling,
- Performing fundamental electrochemistry,
- Creating innovative devices,
- Researching advanced fuel processing,
- Performing durability studies, and
- Training technicians and researchers in the domestic fuel cell industry.

The program has developed breakthrough thin-film electrode technology which has reduced the amount of platinum required per peak kilowatt by a factor of more than 20 while simultaneously increasing the power density of low-temperature fuel cells. Other program successes include

- Improving fuel cell tolerance to impurities in the fuel stream,
- Improving water management and flow-field/bipolar plate design,
- Developing critical fuel processing components and processes, and
- Optimizing fuel cell design and performance through new understanding and models.

The Impact: Hydrogen-Based Transportation and Power

These advances have enhanced the viability of fuel cells for transportation. They have also enabled low-temperature fuel cells to be considered for a broad range of consumer applications including cell phones, laptop computers, portable power, and residential and industrial combined heat and power systems. Ultimately, this work at Los Alamos can help enable a transition to a renewable, emission-free hydrogen economy.

Hydrogen Fuel Cells for Common-Use Batteries

The Challenge: Cheap, Clean, Long-Life Batteries

Conventional batteries used for portable computers, cell phones, flashlights, radios, and wheelchairs are expensive, short-lived, and environmentally unfriendly. Consumers are demanding energy sources that allow longer service without recharging or replacement and that have a longer shelf-life for applications such as flashlights and radios. Fuel cells could provide the long-lived, clean technology ideal for everything from toys to laptops but have traditionally been too complicated and expensive to be practical.

Air-Breather Fuel Cell Stack

Los Alamos Innovation: The Air-Breather Fuel Cell Stack

Following its long and successful history of working with U.S. industry to commercialize hydrogen and fuel cell technologies, Los Alamos recently teamed with Enable Fuel Cells Corporation through a cooperative research and development agreement under the DOE Hydrogen Program. Together, Los Alamos and Enable Corp. have developed the breakthrough Air-Breather Fuel Cell Stack technology.

The Air-Breather combines hydrogen and oxygen to produce electricity and water with zero emissions. Unlike its water-hungry predecessors, the Air-Breather (via its membrane electrode assembly) forces water to diffuse out and oxygen to diffuse in. This process requires less humidification and is more water-efficient.

Fuel-cell systems using Air-Breather technology are small, simple, rugged, and inexpensive. They produce only electricity and clean water with no need for additional cooling, reactant compression, or humidification.

Real-world applications of the Air-Breather technology have been tested with good results. These include (1) extending power to the few hundred-watt level, (2) demonstrating a complete power system on a personal mobility vehicle (a 3-wheeled scooter typically used by the elderly or infirm), and (3) commercially licensing to Enable Corp. the technology for battery replacement.

David Garman, right, Department of Energy Assistant Secretary for Energy Efficiency and Renewable Energy, listens as Mahlon Wilson of Electronic and Electrochemical Materials and Devices describes how a hydrogen-powered fuel cell works to power a personal mobility vehicle.

The Impact: Common Use of Hydrogen Fuel Cells

Hydrogen fuel cells can become the energy source for a host of small-scale applications. Several industries have expressed interest in applying Air-Breather technology to premium products:

- Entertainment/Recreation—cabins, camping, hiking, and sailing.
- Services—search-and-rescue, police, emergency, and military organizations.
- Industry—communications, navigation, telemetry, and computation in remote or inaccessible locations.

Hydrogen Storage Innovations to Enable Zero-Emission Vehicles

The Challenge: Storing Enough Hydrogen Safely

For nearly two decades, the nation's oil use for transportation has grown at an average rate of 2% per year. Consumption for highway vehicles has reached 10 million barrels per day. In addition to dependence on imported energy, oil use for transportation has major environmental effects, producing 79% of U.S. carbon monoxide emissions, 54% of nitrogen oxides emissions, 44% of volatile organic emissions, and 33% of CO_2 (greenhouse gas) emissions. Hydrogen powered vehicles could help solve these problems.

The FreedomCAR Fuel Cell Technology Team and U.S. Department of Energy have identified hydrogen storage as one of the biggest hurdles to introducing zero-emission hydrogen fuel cell vehicles and thus one of the highest priorities in research and development. Current technologies—including storage approaches based on compressed gas, hydrides, and cryogenic liquids—do not, and are not expected to, reach targets incorporating vehicle range, cost, weight, volume, refueling time and ease, and safety.

Los Alamos Innovation: Chemisorption, Microspheres, and Materials Science

Los Alamos is approaching the hydrogen storage hurdle with a diverse, multidisciplinary group of experts. This team is drawing on Los Alamos's capabilities in materials and surface characterization (including neutron scattering), materials synthesis, and innovative testing and performance characterization methods.

This team's in-depth research and development program for transcending hydrogen storage deficiencies will include investigating (1) chemisorption, (2) polymer microspheres (offering a safe hydrogen storage medium flowing much like a liquid for rapid refueling and storage), and (3) potential storage materials with high-throughput screening and combined approaches.

The Impact: Zero-Emission Vehicles

Breakthroughs in hydrogen storage at Los Alamos could have impacts beyond the transportation sector with other fuel cell applications including (1) battery replacement and portable power for both civilian and military use and (2) buffer hydrogen storage in renewable-energy and fuel-cell power systems.

Los Alamos efforts are likely to improve the technology to store large quantities of hydrogen in a safe, economical, easily-refillable, energy-efficient, compact, and lightweight configuration—all of which are necessary to make zero emission vehicles a reality. This team's success could elevate hydrogen in the U.S. and the world as a flexible, secure, domestically-produced, and clean energy source.

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Fuel Processing for Fuel Cell Systems

The Challenge: Developing New Sustainable Power Technologies

Our energy, environmental, and economic security are challenged by current technologies for power production in transportation, buildings, and industry. To achieve the vision of flexible, affordable, safe, domestically-produced energy to be used in all sectors of the economy and in all regions of the country, the nation needs new power technologies that reduce resource depletion and negative environmental impacts.

Los Alamos Innovation: Integrating Strong Hydrogen Programs into Industry Applications

With nearly 30 years of experience in hydrogen and fuel cells, Los Alamos has been identified by the U.S. Department of Energy as its premier laboratory for hydrogen and fuel cell R&D. Promising developments in power technologies for hydrogen generation at Los Alamos are currently being sponsored by DOE's Office of Energy Efficiency and Renewable Energy and directed by DOE's Office of Hydrogen, Fuel Cells, and Infrastructure Technologies. Los Alamos has also earned an international reputation for scientific and engineering excellence and innovation for two aspects of its work: (1) performing fundamental research to improve the performance and durability of low-temperature fuel cells while simultaneously lowering the cost; and (2) developing fuel processing and associated cleanup technologies to allow hydrogen fuel cells to run off hydrogen-rich gas streams derived from hydrocarbon fuels.

The cylinder to the left is a preferential oxidation (PrOx) unit connected to a laboratory test apparatus.

In collaboration with U.S. industry and driven by a commitment to advance multidisciplinary approaches, Los Alamos has achieved the following technology advancements:

- Preferential Oxidation (PrOx) technology and cleanup approaches—transferred to the domestic fuel cell industry for demonstration purposes and now being applied to other fuel-stream trace impurities that cause fuel cell degradation.
- Fundamental modeling and *in situ* characterization techniques—advancing the prospects of even difficult-to-reform fuels such as diesel.
- A significant DOE program to determine the effects of individual fuel components and additives on reforming to help develop a future liquid hydrocarbon fuel for fuel cells.
- An established fuel cell durability program where test cells are operated on real reformate to determine fuel and fuel-processing effects on lifetime and performance.

Features of the pioneering technology at Los Alamos in fuel reformation and cleanup can be found in most, if not all, fuel processing systems for both stationary and transportation fuel cells under development worldwide.

The Impact: Emission-Free Power for a Secure Energy Future

With strong future programs virtually assured, the technologies advanced by Los Alamos can enable distributed heat and power generation from diverse domestic resources and improve the efficiency of energy conversion. This will enable a transition to a renewable hydrogen economy with emission-free power, and greatly improve national energy, environmental, and economic security.

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Direct Methanol Fuel Cells for Portable Electronics

The Challenge: Overcoming Conventional Battery Deficiencies

Many portable electronic devices on the market today require increasing power, but they continue to use conventional batteries that are expensive, short-lived, and environmentally unfriendly. In some applications, such as emergency portable electronics, battery shelf-life can be a problem.

There is significant market pull for batteries that will allow longer service without recharging or replacement. Fuel cells could provide the long-lived, clean technology ideal for portable electronic devices, but in the past they have been too complicated, expensive, and inefficient to be practical. While hydrogen fuel cells offer appropriate power density, with current technology, adequate energy storage is a problem at low power levels.

Los Alamos Innovation: Direct Methanol Fuel Cells

In an effort to overcome these deficiencies, Los Alamos is developing Direct Methanol Fuel Cell (DMFC) power systems. This project uses the capabilities and expertise developed in more than 20 years of fundamental research and proof-of-concept device development in polymer electrolyte membrane fuel cells at Los Alamos. This work is funded by the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy through its Office of Hydrogen, Fuel Cells, and Infrastructure Technology.

Los Alamos has performed fundamental research and has developed innovative DMFC power systems that are simpler, smaller, lighter, and more affordable, efficient, and reliable. Laboratory advances have leveraged improvements in materials, structures, operating conditions, and supporting systems and components to largely resolve the performance issues.

Los Alamos has a long and successful history of working with U.S. industry to commercialize fuel cell technologies. Early commercial applications of DMFC technology could include power for cell phones, portable computers, personal digital assistants, and multimedia players. Supported by the DOE, Los Alamos has teamed with Motorola to develop and commercialize DMFC technology at the sub-watt to few-watt levels and licensed its DMFC intellectual property portfolio to MTI Micro Fuel Cells.

Motorola cell phone powered by a direct methanol fuel cell.

The Impact: Wide Use of Portable Fuel Cells

The innovation and discoveries in methanol fuel cells also support hydrogen fuel cell research and development at the Laboratory to the betterment of both. Future advances are expected to make DMFC's cost-competitive while offering energy density unavailable from batteries. DMFC's may well be one of the first fuel cell systems to penetrate the market and reach volume production. Since they share many materials and features with hydrogen-fueled systems, the commercialization of direct methanol fuel cells will facilitate commercialization of hydrogen systems.

Direct Methanol Fuel Cells for Portable Power

The Challenge: New Power Sources for Defense Applications

The U.S. Department of Defense needs lighter and more compact electric power sources for soldiers, robotics, and other emerging applications. The primary and rechargeable batteries currently used for these systems store an insufficient amount of energy to meet the needs of critical future missions.

Two 11-watt fuel cell stacks (above), developed at Los Alamos, are at the core of the DMFC-20 power system (below). The box to the left of the laptop contains fuel for the fuel cells housed in the larger box to the right. This system has up to 10 times the energy density of batteries.

Los Alamos Innovation: Breakthroughs in DMFC Technology

The Defense Advanced Research Projects Agency's (DARPA) Palm Power Initiative has funded Los Alamos to develop the science and technology base for a palm power demonstration based on the Laboratory's direct methanol fuel cell work. This project applies capabilities and expertise developed during more than 20 years of fundamental research at Los Alamos, research that has generated many proof-of-concept devices in polymer electrolyte membrane fuel cells.

While past direct methanol fuel cells have had relatively poor performance, Los Alamos has largely solved the problems with technical innovations in membrane materials, catalyst formulation, electrode structures, methanol dilution, and operating temperature. The result is a simple, rugged DMFC that

- Directly oxidizes the high-energy-density hydrogen carrier at the fuel cell anode;
- Allows both high-energy density and rapid refueling and reuse;
- Exceeds the capabilities of traditional fuel cells in size, affordability, and efficiency;
- Adjusts to the desired power characteristics of specific applications; and
- Provides stable and reliable performance with a relatively simple system design.

The high energy density and environmentally benign construction of the DMFC provide distinct advantages over most battery technologies. Further advances are expected to make these systems scalable to higher power levels, like the higher power DMFC portable power systems previously developed by Los Alamos and Ball Aerospace for the Department of Energy in collaboration with the U.S. Army Communications and Electronics Command (CECOM).

The Impact: Compact, Reliable Portable Power

Early applications of DMFC technology include (1) meeting the portable power needs of the military, intelligence community, police, and other emergency organizations; and (2) serving as dependable, long-lived sources of industrial electricity for communications, navigation, telemetry, and computation in remote or inaccessible locations. Future DMFC power systems may become as ubiquitous as batteries are today.

Future Directions

Trends and Issues

Concerns with current energy use patterns are rapidly increasing national interest in energy sustainability. Two great concerns are (1) threats from the environmental effects of toxic emissions and greenhouse gases and (2) economic and security vulnerabilities from reliance on imported oil. Alternative energy systems like those based on hydrogen and fuel cells are enjoying both increased press attention and further scientific consideration.

Goals

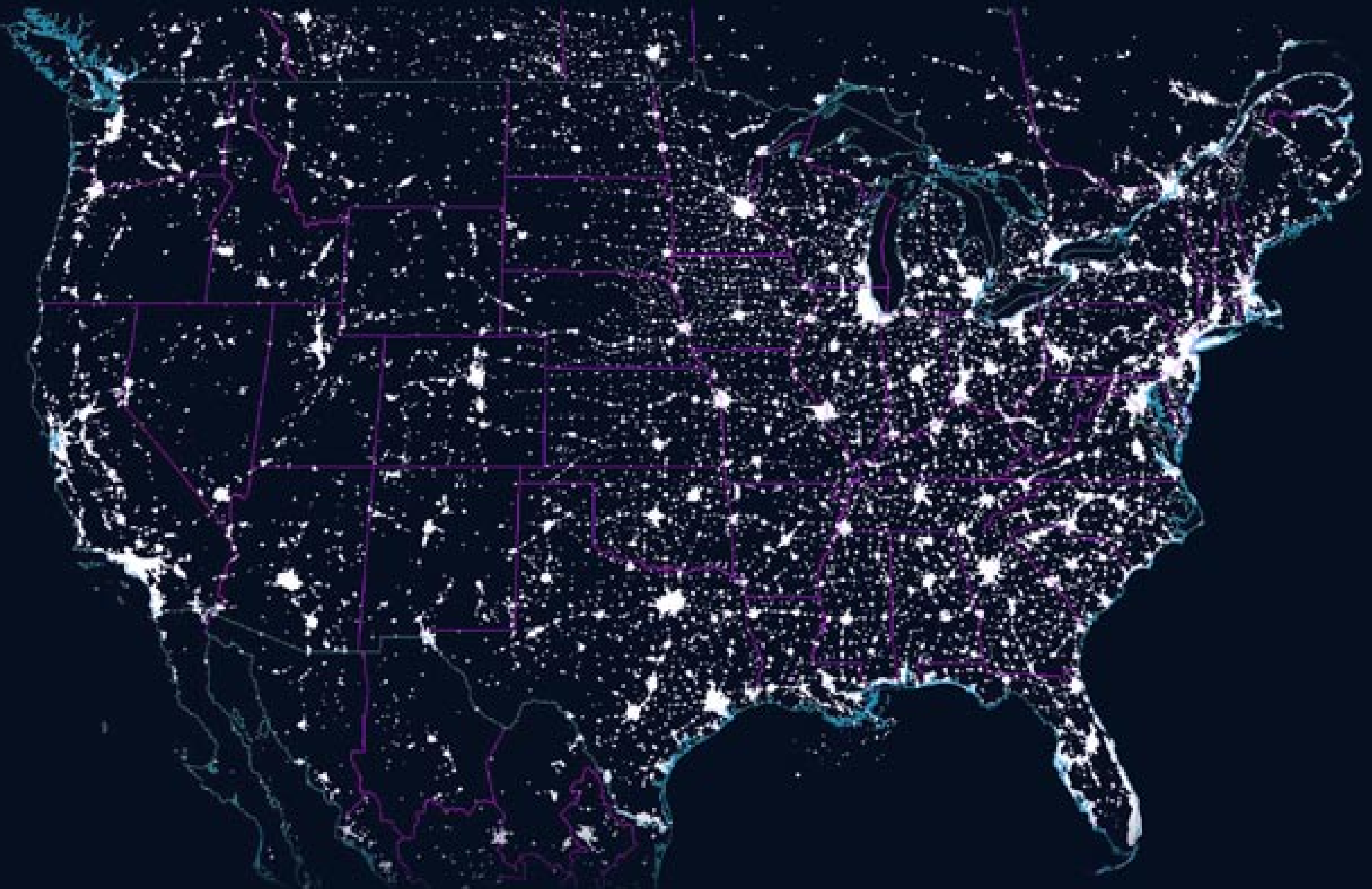
Los Alamos is developing a new national initiative to secure and maintain U.S. dominance in hydrogen and fuel cell technology. With the support of the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy (DOE/EERE), the Laboratory will systematically attack challenges in fuel cell technology. Through collaborations with other national laboratories, universities, and industry, Los Alamos will focus on fuel cell research, application, development, education, training, and enabling technologies in hydrogen production, purification, storage, and safety. These efforts will directly support DOE/EERE goals by enabling a public private partnership that will

- Advance fuel cell technology;
- Develop and validate hardware;
- Train a workforce to meet future fuel cell research and development demands;
- Accelerate implementation of fuel cell technology to meet domestic needs;
- Significantly advance the timeframe for market introduction of fuel cells; and
- Keep the U.S. ahead of foreign competition.

Capabilities and Vision

Successful development of innovative technologies is most likely where cornerstone technology and dedicated technical staff already exist. Fuel cell research and development at Los Alamos has the benefit of a world-class reputation and research portfolio as well as its ability to address the key trends facing hydrogen and fuel cell research in the 21st century. The Laboratory has unparalleled research power and proven success in

- Electrochemical materials and devices,
- Catalyst design, synthesis, characterization, and testing,
- Observational and experimental methods,
- Theory, modeling, and simulation,
- Multidisciplinary approaches to complex systems,
- Documented knowledge base,
- Polymer electrolyte membrane fuel cell research and development,
- High-performance computing, and
- Collaborations with key U.S. industry leaders.



INFRASTRUCTURE

Energy and Environment Compendium

Los Alamos
NATIONAL LABORATORY

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Infrastructure Research at Los Alamos National Laboratory

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LALP-04-026

Infrastructure Research at Los Alamos National Laboratory

Los Alamos National Laboratory performs basic and applied research to secure the nation's energy infrastructure. Central to this research is the development of large-scale, detailed computer models of energy industries and other infrastructures. Such work requires close cooperation with physicists, engineers, mathematicians, statisticians, computer scientists, and economists. Our macro models and micro simulations aim to quantify the physical, operational, and economic behavior of energy networks (electric power, natural gas, oil, and coal generation/transmission/distribution) and non-energy infrastructures important to energy security (transportation, water, communications, and public health). Often these models are combined within interdependency, optimization, and risk assessment frameworks.

Current Research Activities

Los Alamos is developing and testing new technologies for the next generation of electrical grids. These new technologies will require integration into a complete architecture including hardware solutions as well as modeling, simulation, and data analysis. The new programs supporting the next generation electrical grid must sense the health of the grid and input this data into the models and tools under development. The Laboratory is participating in the governance of DOE's Energy Infrastructure Training and Analysis Center (EITAC) through a steering group that includes Sandia and Argonne national laboratories. The first EITAC visualization capabilities will be Los Alamos products.

Current Research and Development Challenges

- Development of robustness metrics when multiple infrastructures are mutually dependent.
- Models and simulations that predict and visualize energy outages based on loss of critical components.
- Communication protocols and data aggregation techniques to support a real-time visualization and forecasting capability.
- Analysis of emerging technologies that could be applied to the national electric power grid to help minimize large scale outages (would be used to help determine specifications and investment priorities for future technologies).
- Development of tools to perform real-time, short-term dynamic analysis of the national electric power grid.
- Development and application of technologies, such as high-temperature superconductors, to reduce or eliminate the present bottlenecks in the electric power system.

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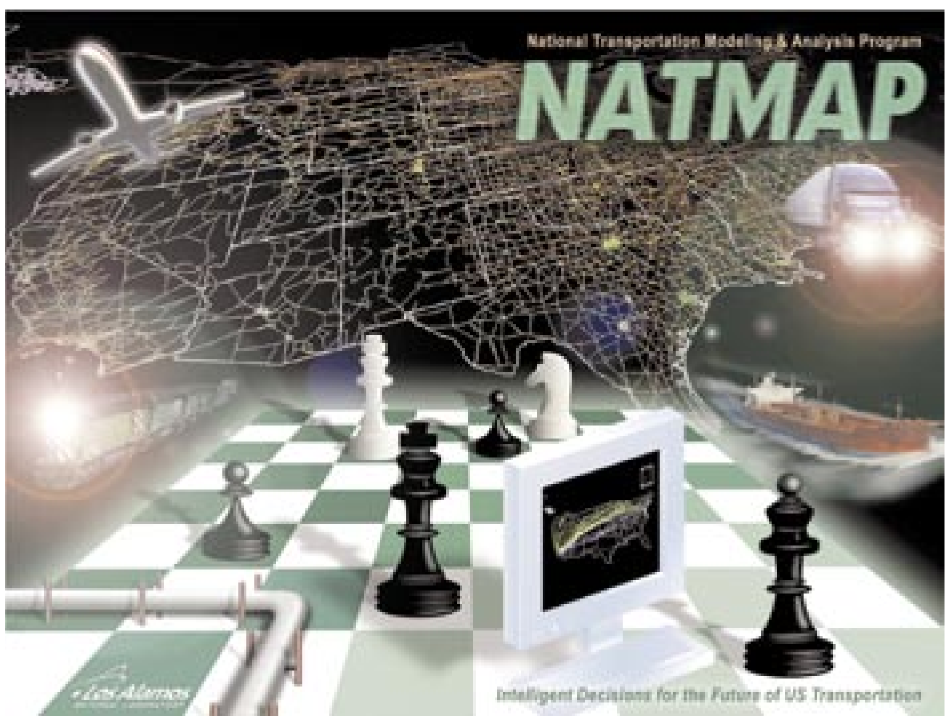
National Transportation Modeling and Analysis Program

The Challenge: Simulating Transportation of Commodities

Our nation's fossil energy infrastructure is highly dependent on the transportation infrastructure. Without the shipping, trucking, pipelines, and rail systems that move fossil fuels, the U.S. energy system would come to a halt. The National Transportation Modeling and Analysis Program (NATMAP), currently under development at Los Alamos with the sponsorship of the Department of Transportation, is simulating the many modes of the national transportation system to understand their dependencies and vulnerabilities. NATMAP models the transportation network down to the fine detail of individual carriers—such as trucks, trains, planes, waterborne vessels, and pipelines—to simulate commodity shipments across the U.S. infrastructure. It also simulates the movement of individual freight shipments from production areas through intermodal transfer facilities and distribution centers to points of consumption.

Los Alamos Innovation: Making Detailed Representations of Traffic Flows at Many Different Levels

Unlike traditional, static models that can only model transportation and flows at gross levels, NATMAP employs dynamic, “bottom-up,” disaggregated modeling techniques. The advantage of this individual carrier/shipment simulation approach is in the level of detail in which the nation’s fossil fuel transportation system can be represented, from trucks and goods moving among counties and within regions, to national multi-modal traffic flows including cross-border trade with Mexico and Canada. This strength can be exploited for transportation policy and for security and infrastructure investment purposes.



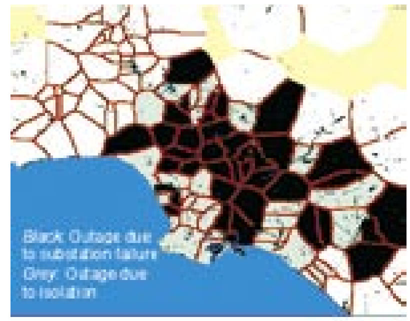
The Impact: An Efficient and Secure Transportation Infrastructure

Initial deployment will focus on real-world issues defined by the Department of Transportation and other stakeholders, thus enabling intelligent decisions that will ensure the future efficiency, reliability, and security of the transportation infrastructure and the economy it supports.

Electric Power Grid Modeling

The Challenge: Securing the Energy Infrastructure of the United States

Los Alamos National Laboratory researchers have long investigated energy generation and transmission networks to help various federal, state, and local agencies to understand these infrastructures, track their evolution, identify their strengths and weaknesses, assess their reliability, and analyze their economics. With extensive databases, tools, and expertise, the Laboratory has taken a two-pronged approach by studying (1) the effects of electric power industry deregulation and mergers, and (2) the effects of natural disasters on the energy infrastructure of the United States.



Projected (simulated) electrical outage in the Los Angeles area due to Earthquake damage.

Los Alamos Innovation: Simulating Economic and Physical System Connections

Los Alamos has made innovative simulations of the interdependencies between energy infrastructures and deregulated energy markets in an attempt to better understand market structure influence on day-to-day systems operation. The Laboratory has also evaluated air quality and economic tradeoffs between centralized and dispersed electric generation plants. State-of-the-art power flow simulation tools are used to identify

- service and outage areas,
- outage duration,
- critical system components,
- restoration strategies,
- mitigation options, and
- system performance.

These analyses determine the electric grid's ability to meet electrical demand and energy requirements. Los Alamos has developed a unique, in-depth capability to collect the required data, build and verify accuracy of infrastructure models, and integrate these into databases describing the national infrastructure. From urgent case studies to long-term research projects, work has been coordinated with other national laboratories, industry, and government agencies.

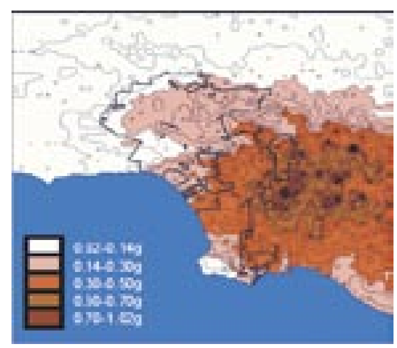


Illustration of damage estimate based on previously estimated ground motion for a simulation scenario.

The Impact: A More Reliable Power Infrastructure

The main goal of this research activity is to identify outage events that impact electric power supply reliability, develop vulnerability mitigation options, and create business continuity strategies.
By foreseeing potential vulnerabilities caused by market changes or natural disasters, potential problems can be addressed before they interfere with the nation's economy and quality of life.

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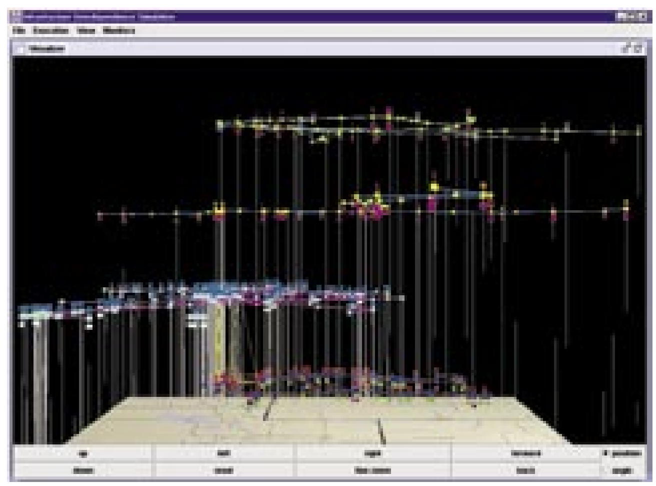
Interdependent Energy Simulation System

The Challenge: Understanding System Interdependencies

The nation's security requires that the interdependent energy, communication, and transportation infrastructures provide an appropriate quality of dependable service. Each of these infrastructures consists of many interlinked subsystems. To accurately simulate the nation's energy infrastructure, Los Alamos National Laboratory has expanded its efforts in electric power grid security to include energy generation and transmission subsystems. We have modeled natural gas pipeline networks and petroleum liquid networks and also plan to model the U.S. coal infrastructure. Energy infrastructures typically have feedback loops, where infrastructures depend upon each other to deliver their products. For example, a gas-fired electric generating plant requires a steady supply of natural gas, and the natural gas pipelines may require electric-powered compressors to maintain sufficient pressure. The interdependency concept is critical to understanding these complex coupled systems, and an inflexible modeling and technology base has hampered the understanding of them in the past.

Los Alamos Innovation: Coupled Models of Complex Infrastructures

The Interdependent Energy Infrastructure Simulation System (IEISS), embodied as analysis software tools developed at Los Alamos in collaboration with Argonne National Laboratory, aims to develop a comprehensive simulation study of the nation's interdependent energy infrastructures to address a wide variety of intra- and inter-infrastructure dependency questions. This capability allows the Laboratory to identify and understand infrastructure interdependencies during normal operations and disruptions and provides the ability to assess the technical, economic, and national security implications of system configurations. This will enable a detailed analysis and understanding of entire interdependent infrastructures, including their components and couplings, in a manner far beyond what could be done previously.



A prototype version of IEISS was used in preparation for the 2002 Salt Lake City Olympics. This figure overlays major energy infrastructure networks on a map of key Olympic sites. Vertical lines identify system interdependencies.

The Impact: Avoiding Crises by Identifying Weaknesses

Los Alamos envisions diverse applications for analyses based on IEISS. The ability to identify critical components and vulnerabilities in coupled infrastructure systems will allow us to (1) assess how future investments in the systems might affect quality of service; (2) perform integrated cost-benefit studies; (3) evaluate the effects of regulatory policies; and (4) aid in decision-making during crises.

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Urban Security

The Challenge: Protecting Cities

Recognizing the importance of understanding the social, economic, infrastructure, and environmental components of cities in an integrated manner, Los Alamos National Laboratory began work on the Urban Security Project. The majority of the world's population now resides in cities that are increasingly the foci for epidemics, warfare, and terrorism. Large cities are places where infrastructure and environment meet humanity, creating a situation ripe for natural disasters of grand scale, as well as human-made disasters that often result from poor long-term planning decisions.

Los Alamos Innovation: Coupling Human, Engineered, and Environmental Systems

Using the broad spectrum of disciplines and computing capabilities at Los Alamos, the Urban Security project examines the links between human society, the economy, infrastructures, and the environment. By working collaboratively across the physical and social sciences to more fully understand human, engineered, and natural systems, we can more effectively prepare for natural disasters through hazard mapping, natural process modeling, and crisis forecasting and planning. New tools will be developed for long-range urban planning, and vulnerability to terrorism or large-scale mischief will be identified.

The Impact: Safer, Well-Managed Cities

The 21st century will call for the increasing collaboration of physical and biological scientists with social scientists, economists, and infrastructure engineers. With the existing expertise to fully develop an urban science mission, the interdisciplinary and interdivisional spirit of the Laboratory could be used to research and develop homeland security solutions and to address urban planning problems such as the effects of natural hazards, uncontrolled urban growth, unstable bureaucracies, environmental security, and cost-effective urban planning. Research and development can result in new approaches to city planning, management, and decision-making, and tools can be developed to monitor change. Finally, virtual training environments can be developed for city managers, emergency responders, and utilities engineers.

Lower Manhattan following the terrorist attacks on 9/11/2001.

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Urban Dispersion Modeling of Airborne Chemical and Biological Agent Threats

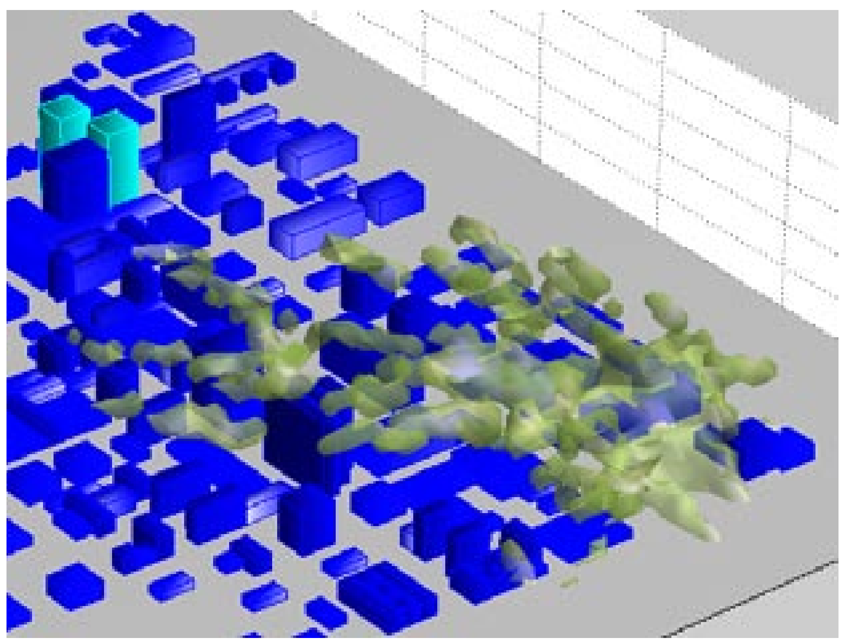
The Challenge: Responding to Chemical and Biological Terrorism

Because one possible terrorist attack scenario involves the release of Chemical or Biological (CB) agents in a city, Los Alamos National Laboratory has been working on urban plume transport and dispersion modeling under the DOE Chemical and Biological National Security Program (CBNP) and the Department of Homeland Security. Most dispersion models currently in use for emergency response applications take little or no account of the urban setting. Without incorporating the presence of buildings, the dispersion of a CB agent released in an urban area is difficult to predict.

Los Alamos Innovation: Developing Fast Response Models For Use in Cities

To simulate the transport and dispersion of a CB agent in urban areas, Los Alamos is developing fast response models that will compute the three-dimensional wind patterns and dispersion of airborne contaminants around clusters of buildings. These types of models are essential for vulnerability assessment studies where many cases must be simulated in a limited amount of time or when an answer is needed quickly. The Quick Urban & Industrial Complex (QUIC) fast-response urban dispersion modeling system includes the QWIC-URB wind model and the QWIC-PLUME dispersion model. In addition, a hybrid engineering and meteorological computational fluid dynamics model called HIGRAD is being used for high-fidelity applications. These codes are intended to

- formulate scenarios for tabletop exercises;
- plan strategies for coping with emergencies at special events; and
- develop vulnerability analyses and mitigation strategies for specific sites.



Simulation of a chemical or biological agent dispersion through downtown Salt Lake City using the QUIC dispersion modeling system. Calculations took approximately 5 minutes on a PC laptop.

The Impact: Being Prepared for Real-World Emergencies

Models developed for this project have already been applied to real-world scenarios. They have contributed to three important homeland defense programs—the National Biological Defense Initiative, the Biological Aerosol Sentry Information System, and Project BioWatch. Vulnerability assessments have been performed for government facilities after 9/11 and for the Safety Division at Los Alamos. The program has also contributed to the development of a guide, the *Emergency Responder's Rules-of-Thumb for Toxic Airborne Releases in Cities*, that has been distributed by FEMA, incorporated into police training courses, and used by fire chiefs and state agencies.

ElecNet

The Challenge: Preventing Power Outages and Electrical Accidents

As we have become more and more reliant on electrical power, demand continues to increase beyond the infrastructure's capacity to supply, and power outages are commonplace. Annual losses caused by power outages total in the billions of dollars. In addition to outages, power efficiencies are much lower than they could be, resulting in waste and higher costs for electricity.

Beyond monetary losses resulting from problems with electrical power reliability and efficiency, there is the issue of human safety. A huge percentage of annual fires, property losses, deaths, and injuries, can be attributed to electrical accidents.

Los Alamos Innovation: ElecNet's Intelligent Sensors that Detect and Prevent Problems

ElecNet is a smart, secure, networked system that can monitor important electrical and security data in real time. ElecNet is easily scalable and can provide rapid alarming and control from small to large networks. For example, power and sensor status could be communicated quickly, inconspicuously, and securely between an emergency operation center and a nuclear facility. With ElecNet, sensors are embedded into electrical devices such as light switches, electrical outlets, and circuit breakers. These electrical devices are networked together so that sensor data from devices and circuits can be monitored and summarized elsewhere. ElecNet's many diagnostic capabilities include monitoring circuit loads, detecting arcs, and sensing fire and heat. The system also has microprocessor intelligence that allows alarming and automatic control to be incorporated into the system.

Prototypes of ElecNet electrical outlet and switch.

The Impact: Safer and More Efficient Electrical Networks

Effective monitoring and networking of electrical devices and circuits can facilitate earlier detection of problems and prevent accidents or equipment damage. The ElecNet system can alert users to problems, or it can actually shut down a circuit or outlet to prevent injury, death, or equipment damage. Since ElecNet has embedded intelligence, it can automatically decide to cut off power to a device or circuit when it is not required to improve electrical efficiencies. ElecNet's networking and embedded intelligence abilities allow data to be moved and reported in rapid and meaningful ways.

High-Temperature Superconductors

The Challenge: Upgrading the Reliability and Efficiency of the Nation's Electric Power Infrastructure

Ten percent of electricity generated in the U.S. each year (300 million kilowatt hours) is lost due to resistance of the copper and aluminum wiring currently used to transmit power across the nation's electrical grid. The energy lost is enough to supply the combined energy needs of New Mexico, Arizona, California, and Oregon. Superconductors, materials that have no electrical resistance when cooled with liquid nitrogen, can carry up to 100 times the electricity of ordinary copper or aluminum wires of the same size. These materials can be used in many electric power applications, such as transmission lines, industrial motors and generators, fault-current limiters, and transformers. The key to applying superconductivity to energy security is developing a strong and flexible high-temperature superconducting wire capable of carrying large currents in magnetic fields. At Los Alamos, this objective has led to two parallel efforts that focus on two different superconducting compounds known as BSCCO and YBCO.

Electrical transmission lines are one of the many uses of high-temperature superconductors.

Los Alamos Innovation: Advancing Superconductor Technology for Practical Application

The first technique to yield good superconducting wire was the oxide-powder-in-tube method in which oxide powders of BSCCO are loaded into silver or silver alloy tubes, sealed, and then drawn or extruded into round wire. The round wire is then thermally processed to form a superconducting composite, or it is further rolled to produce a flat tape which is then thermally processed to produce a superconductor. Most of the conductors produced with the BSCCO materials are made in the tape form. To date, the only practical, long lengths (>1 km) of superconductors have been made with BSCCO materials. These conductors are closer to commercialization than the YBCO conductors.

YBCO conductors, known as "coated conductors" or "second generation" wires, promise better performance in high magnetic fields, higher temperature operation, and lower cost compared to BSCCO wires. However, the drawing and rolling technique for producing BSCCO wire does not work well for YBCO wire, so Los Alamos has developed new techniques to produce practical lengths of YBCO wire. The new techniques rely on ion beam assisted deposition and pulsed laser deposition to deposit thin films of YBCO on a strong and flexible substrate.

Reels of superconducting tape that have a current density 100 times that of copper wire.

To advance these technologies and move them quickly out of the laboratory to the electric grid, Los Alamos established the Superconductivity Technology Center, a user research facility that coordinates a multidisciplinary program in research, development, and technology transfer in collaboration with industry, universities, and other national laboratories. Research areas include wire and system development, powder synthesis, processing of tapes and coils, deposition of thin and thick films, characterization of micro-structural and superconducting properties, power cryogenic engineering, and fabrication of prototype devices. Through industrial collaborations, more than 1,000 km/year of BSCCO wire are now being manufactured.

The Impact: Unprecedented Electrical Efficiencies and Cost Savings

Superconductivity will have a dramatic economic impact. The electricity saved by superconductor cables could equal $4 billion per year. In comparison to conventional technologies, superconductivity power equipment will typically be half the size and have half the energy losses. High-temperature superconductors will dramatically enhance the nation's energy security by increasing the efficiency and reliability of the electrical power grid.

Superconducting Fault Current Limiters

The Challenge: Preventing Power Outages and Damage from Current Surges

Lightning strikes a transmission tower, high winds blow down a tree, a truck runs into a power pole, heavy ice pulls down power cables, a careless builder digs up underground power lines, an unfortunate squirrel is in the wrong place at the wrong time; all of these are familiar and common occurrences. And all of them can cause current surges, or "fault currents," to travel through the electric grid at up to 20 times the normal operating current and cause blackouts. The result, in addition to the temporary inconvenience of being without power, is billions of dollars in damage to utility, industrial, and homeowner equipment, and in lost business time and manufacturing production. In over a century of electric power, no economical and efficient current surge suppressor, or fault current limiter, has been devised for the electric power grid. Superconductors are poised to change that.

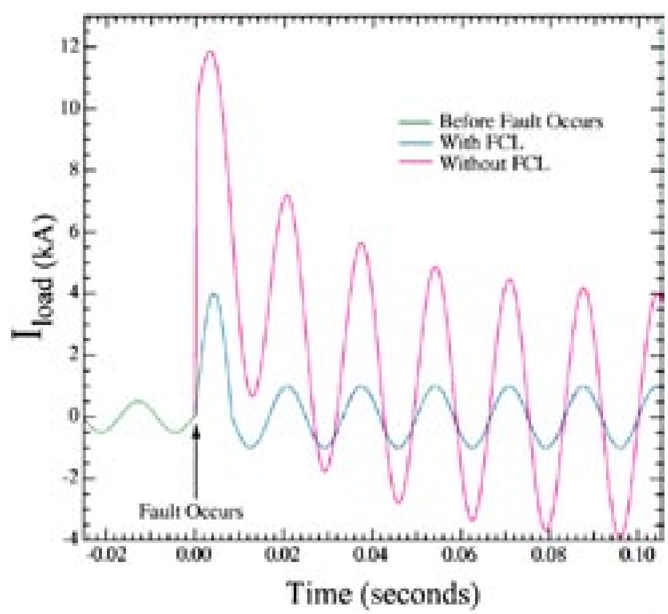
Lightning is only one of many causes of fault currents that result in blackouts and costly damage to electrical equipment.

Los Alamos Innovation: Applying Superconductivity to Fault Current Limiter Technology

A perfect fault current limiter (FCL) should (1) have zero impedance during normal operation; (2) increase greatly in impedance when excessive current is present; (3) rapidly detect surges and act instantly; (4) allow immediate return to normal operation after the fault has cleared; and (5) be fully automatic, reliable, and inexpensive. These are precisely the characteristics of high-temperature superconductors. Because superconductors normally have zero impedance, a superconducting FCL would be "invisible" under regular operating conditions and not affect efficiency like some FCL devices currently in use. However, the unique properties of superconducting materials cause them to become naturally more resistive when higher currents are present. Unlike circuit breakers, which may not open before damage has occurred and may not reclose if the fault current was too severe, a superconducting FCL will instantly react to control a fault current and then return to normal operation just as quickly after the fault has passed.

Los Alamos National Laboratory has long been an international leader in the science and technology of high-temperature superconductors and has already successfully applied its expertise to the control of fault currents. In collaboration with General Atomics, IGC-SuperPower, and Southern California Edison, Los Alamos has developed and successfully tested a 15 kV fault current controller that combines advanced power electronics with the world's largest superconducting solenoids. The Laboratory is now working with IGC-SuperPower to create a much simpler, more compact, and less expensive superconducting FCL that can be widely dispersed throughout utility transmission lines. Los Alamos will play a key role in materials characterization, cryogenic engineering, prototype design and fabrication, computer modeling of system performance, and device testing.

The graph shows how superconducting fault current limiters prevent severe spikes following a fault event and stabilize the current rapidly.



The Impact: A Reliable, Uninterrupted Power Supply

Superconducting fault current limiters will greatly increase the efficiency and reliability of the nation's electrical power grid. They will improve safety, enhance power quality, and reduce damage to utility and customer equipment. They will also defer the urgent need for costly transmission and distribution system upgrades by protecting the current aging systems.

NUCLEAR

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Nuclear Technology and Applications Research at Los Alamos National Laboratory

Nuclear Energy Research at Los Alamos National Laboratory

Los Alamos conducts research in both nuclear fission and nuclear fusion. Nuclear fission achieves energy release by splitting heavy atoms (as in a present-day nuclear reactor), whereas nuclear fusion achieves energy release by combining light atoms (as in the process occurring in the core of a star). The Nuclear Technology and Applications Program leads the fission effort while fusion research is managed by Nuclear Fusion Energy Sciences.

Nuclear Technology and Applications Research

Technology development programs carried out within the Nuclear Technology and Applications portfolio aim at major national and international needs, including

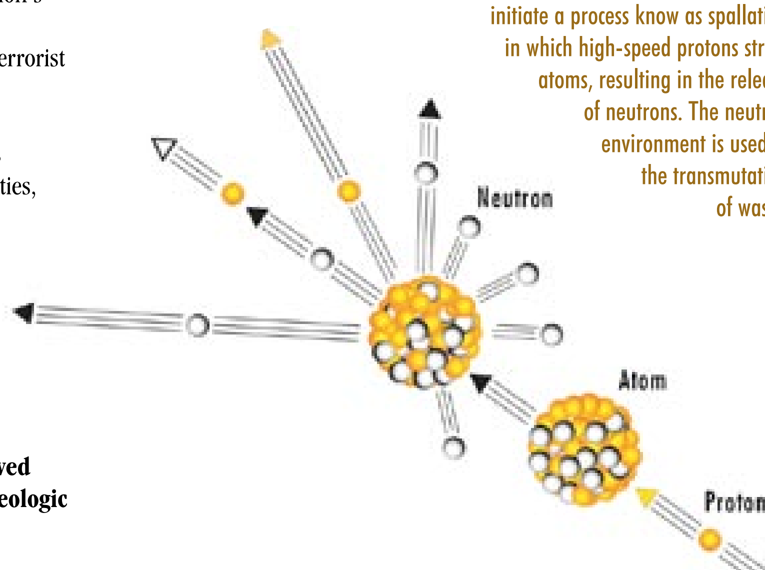
- New nuclear energy technology that supports the goals and objectives of the President's National Energy Policy;
- Technologies that support recommendations on advanced nuclear fuel cycle development made by the directors of six leading Department of Energy national laboratories to the Secretary of Energy;
- Near-term space exploration missions that require significant levels of electrical power for their success;
- Radioisotopes needed nationwide for disease diagnostics and treatment;
- Efforts to ensure continued highest levels of safety of the nation's 100 operating reactors; and
- Efforts to maximize the security of nuclear reactors against terrorist attack or sabotage.

The nuclear technology development and applications efforts at Los Alamos support these efforts through combinations of unique facilities, demonstrated nuclear materials capabilities, sophisticated nuclear system design, and safeguards expertise.

Current Science and Technology Challenges in Nuclear Technology and Applications Research

- **New technology systems to effectively deal with long-lived radionuclides in nuclear waste that drive long-term geologic disposal requirements**—Developing and demonstrating efficient technologies that separate plutonium and higher actinides from used fuel discharged from power reactors and that effectively use recovered materials in reactor or accelerator-based nuclear systems to minimize through transmutation of nuclear waste long-lived radionuclide inventories, that would otherwise be discharged to the environment, are equally important components of meeting this challenge.
- **New technologies to ensure nuclear fuel cycle and reactor systems deployed for future energy needs exhibit highest levels of proliferation resistance**—Integrating and optimizing technologies *a priori* for nuclear materials safeguards and nuclear materials separations represent development approaches that are needed to meet this challenge.
- **Sophisticated analysis capabilities to understand nuclear energy contributions to future national and global energy sustainability**—Understanding end-use scenarios and technology competitiveness, achieved through energy-environment-economics simulation tools, can guide nuclear energy technology development.
- **Increased production of radioisotopes required for medical and scientific applications**—Meeting the challenge with a new Isotope Production Facility at LANSCE and plans for new, dedicated accelerator facilities can meet this challenge.

A proton accelerator can be used to initiate a process know as spallation in which high-speed protons strike atoms, resulting in the release of neutrons. The neutron environment is used in the transmutation of waste.



- **Reliable and safe production of nuclear energy for space applications are required by NASA for upcoming missions to Mars and the Jovian moons**—Designing robust space reactors that need no terrestrial nuclear testing, as well as manufacturing appropriate nuclear fuels, will meet this challenge in a safe, cost-effective manner.
- **Threat assessment (safety, terrorist, sabotage) of nuclear facility vulnerabilities is a key need**—Developing sophisticated risk assessment tools and advanced simulation capabilities based upon modern computing environments is the key resource to answer this challenge.

Nuclear Technology and Applications Capabilities

- **Nuclear materials chemistry and separations**—Los Alamos has many scientists in the Chemistry and Nuclear Materials Technology divisions that have a unique combination of innovative process design and operational experience. The Plutonium Facility (TA-55) is a major national resource that allows technology demonstration in nuclear materials environments. Plans by the Seaborg Actinide Science Institute for new facilities available to outside researchers will further enhance this capability.
- **Nuclear fuels production**—Facilities at TA-55 for fuels production are unique in the DOE laboratory complex. Additionally, experimental capabilities are being enhanced by new initiatives in sophisticated simulations for novel nuclear fuels properties and performance.
- **Nuclear system design**—Modeling and simulation using codes such as MCNPX and TRAC contribute to Laboratory researchers' novel design efforts for applications such as space reactors.
- **The Isotope Production Facility and associated hot cell and isotope separations facilities**—The LANSCE-based Isotope Production Facility is the major national resource for producing neutron-deficient radioisotopes. Site-located hot cells and supporting analytical and separation capabilities allow Laboratory scientists to meet external customer needs on a timely basis.
- **Nuclear safeguards technology**—Los Alamos is the only national laboratory with experience in developing and applying nuclear safeguards technology to foreign fuel fabrication, nuclear materials storage, and reprocessing facilities in Russia and Japan.
- **Experimental facilities and theoretical capabilities for nuclear data**—The LANSCE facility is a major U.S. resource for measuring proton- and neutron-induced nuclear reaction cross sections over energy ranges from milli electron volts to hundreds of megaelectron volts. This experimental capability is complemented by an internationally recognized effort in the theoretical analysis and modeling of cross sections and in the creation of computer-based data libraries for use in nuclear design codes.
- **Energy and nuclear fuel cycle modeling**—The Laboratory has developed and applied sophisticated models of the nuclear fuel cycle to examine material flows, economics, and waste disposal requirements for advanced nuclear systems. Such fuel cycle models are also coupled into energy-economic-environment models that allow future energy demand and supply scenarios on national, regional, and global bases to be examined. These models are used to examine the competitiveness of nuclear energy with other options and to ascertain policy impacts such as carbon taxes on fossil fuels on nuclear market shares.
- **Risk and threat assessment**—The Laboratory has decades of history in developing and applying advanced methods for probabilistic risk assessment (PRA). While such PRA methods have been applied to analysis of severe reactor accidents, they are now being applied to nuclear facility safety and security. Complementing PRA methodology development and application has been the creation of sophisticated tools for reactor safety analyses, in particular the TRAC code—a principal resource for the Nuclear Regulatory Commission (NCR).

The LANSCE linear accelerator is being used to develop nuclear data and transmutation science and will soon house a major experiment to further the development of new materials and fuels for the transmutation of nuclear waste.

Nuclear Fusion Energy Sciences

Fusion energy, the process which powers the stars, involves fusing together light atoms to release nuclear energy. It offers the hope of a nearly limitless supply of energy to mankind, with the fuel commonly found in seawater, and has no global warming emissions. Unlike nuclear fission, which happens easily when you stack a pile of heavy metal, fusion reactions are very difficult to ignite on Earth.

At Los Alamos, research into the control of the processes of nuclear fusion began in the early 1950's and continues to this day. Fusion energy research is supported by the DOE Office of Science, Fusion Energy Sciences branch. Our research is conducted along two principal approaches. The first uses powerful magnets to make a "bottle" to contain the hot plasmas, and the second uses inertial compression, either with lasers or ion beams. These are referred to as Magnetic Fusion and Inertial Fusion (see p.15). Learn more about Los Alamos's Fusion Energy Sciences Program at **http://fusionenergy.lanl.gov**.

Transmutation of Nuclear Waste

The Challenge: Addressing Pressing Nuclear Energy and Waste Management Issues

Before additional nuclear power capacity can be developed, the concern for management of nuclear waste produced by commercial nuclear power plants must be addressed. Realizing this necessity, Los Alamos created the Advanced Fuel Cycle Initiative (AFCI) Program to address such pressing nuclear issues as nuclear energy and waste management. As a result, Los Alamos National Laboratory is newly focused on the coordination of expertise, research, and development efforts related to non-weapons nuclear technology and applications. One of the first areas on which the Laboratory is concentrating its efforts is nuclear power.

Los Alamos Innovation: Transforming Radioactive Materials into Less Harmful Substances

With Los Alamos's expertise and research in both accelerator design and target technology, the AFCI Program is developing the technology base for nuclear waste transmutation (the nuclear transformation of long-lived radioactive materials into short-lived or non-radioactive materials), and plans to demonstrate its practicality and value for long-term waste management. The Laboratory has unique capabilities for fuel development for fast and thermal spectrum multipliers, lead-bismuth technology, materials testing, and modeling of advanced separations technologies. Los Alamos has also developed a novel concept for separating uranium from spent nuclear fuel.

Thus far, Los Alamos and its partners have built and operated the front end of a high power accelerator and built and operated a liquid-lead eutectic loop for testing. They have developed and fabricated transmutation (plutonium-nitride) fuels and performed numerous system studies on various waste transmutation schemes to determine the most viable approach to address the nuclear waste issue. And they have obtained nuclear cross-section data and evaluations for isotopes of interest for transmutation.

The Impact: Nuclear Energy as a Safe and Secure Energy Alternative

While the AFCI Program is working on methods to drastically reduce the amount of nuclear waste currently in storage, the goal of the program is to develop the technology that will transition the U.S. into a closed fuel cycle with a more economical and less wasteful use of nuclear materials by reducing the long-term radiological impact of waste and enabling development of a simpler, cheaper repository. This can also reduce proliferation risks, thereby improving long-term prospects for nuclear power.

Uranium (VI) nitrate crystals, part of advanced separations concept for spent fuel recycling. Los Alamos researchers are evaluating a process to crystalize uranium (VI) nitrate from spent nuclear fuel dissolved in nitric acid.

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Isotope Production and Applications

The Challenge: Supplying the Radioisotope Needs of Medicine and Science

Los Alamos National Laboratory is one of three sites that produce and distribute stable and radioactive isotopes for the Department of Energy's Office of Nuclear Energy, Science, and Technology. The radioisotope program at Los Alamos's Neutron Science Center (LANSCE) has been producing radioisotopes for more than 20 years, making it one of the most successful and visible ongoing endeavors in the nationwide production and distribution of isotopes. Without the production capabilities at LANSCE and other national and international facilities, the DOE would not be able to meet the needs of its radioisotope customers. A major milestone was reached in February 2004 with the dedication of a new target irradiation facility at LANSCE for the production of medical research isotopes.

Los Alamos Innovation: Creating Stable and Radioactive Isotopes

Unique radioactive material handling facilities and capabilities in accelerator technology, radiochemistry, chemical processing, and synthetic chemistry allow the Laboratory to offer a variety of products and services. LANSCE and the TA-48 main radiochemistry site hot cell facilities create accelerator-produced isotopes, and the CMR wing 9 hot cell facilities perform chemical processing of reactor irradiated targets. Los Alamos can separate stable and radioactive elements with electromagnetic isotope separation techniques and distribute inventories of americium-241 and other actinides.

The Impact: Meeting the Demand for Commercial and Clinical Radioisotopes

The combination of Los Alamos's unique facilities and radioactive materials handling expertise is essential to this important national program. To ensure the continuing demand for radioisotopes is met, LANSCE is expanding its facilities by designing and constructing a 2-level \$19.9 million Isotope Production Facility that will ensure a dedicated year-round supply of radioisotopes when combined with similar isotope production capabilities at Brookhaven National Laboratory and supplemented by international collaborations. It will also provide significant opportunities for applications at the intersection of the Laboratory’s radiochemistry and biochemistry capabilities. The main customer is the DOE Office of Isotopes for Medicine and Science, but products and services are also distributed to an extended customer base of over 250 institutions, such as hospitals, universities, other research institutions, and industry.

These hot cells in Los Alamos are used to perform chemical separations to isolate and purify the accelerator-produced medical isotopes at LANSCE.

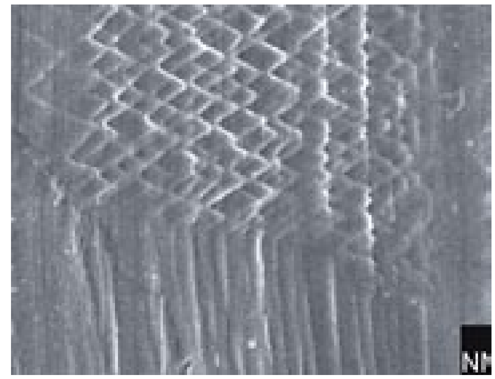
Structural Materials for the Advanced Fuel Cycle Initiative

The Challenge: Identifying Reactor Materials for the Advanced Fuel Cycle Initiative

Reactor materials for the Advanced Fuel Cycle Initiative (AFCI) must withstand high-energy proton and neutron fluxes at temperatures ranging from 400° to 600°C. This project determines the effect of high-energy proton and neutron irradiation on the mechanical properties of structural materials under prototypical conditions of irradiation, temperature, and flux. Prototypic materials are

- Ferritic martensitic steels,
- Austenitic steels, and
- Refractory materials.

The goal is to obtain mechanical properties after irradiation to doses of 200 dpa at temperatures of up to 600°C. The project also addresses materials needs for the Generation IV reactor program with the challenge to push temperatures even higher.



Above: Scanning Electron Microscope (SEM) micrograph showing coarse slip bands on the outer surface of a 316L stainless steel 3 pt. bend specimen after irradiation and testing at 350°C to a dose of 10 dpa in a 570 MeV proton beam.

Los Alamos Innovation: Determining the Effect of High-Energy Proton and Neutron Irradiation on the Mechanical Properties of Structural Materials

Los Alamos is using the following three capabilities to address three key issues:

1. Chemistry and Metallurgy Research (CMR) hot cell capabilities for handling and testing radioactive materials after irradiation in high-energy proton or neutron flux.
2. Atomistic modeling capabilities and expertise to extrapolate the data to conditions not tested experimentally.
3. 800 MeV, 1 mA accelerator for performing some of the materials irradiations.

Below: Los Alamos researchers use a Leitz MM5 Metallograph to view the microstructure of irradiated materials in the CMR hot cells.

The Impact: Managing Nuclear Waste and Designing Advanced Reactors

The ultimate goal of this project is to use the mechanical test data and modeling capabilities to determine structural design allowables for AFCI components. This enables the determination of material lifetimes for specific components in the AFCI program as well as the Generation IV reactor program. Los Alamos has the ability to overcome obstacles in managing nuclear waste and designing advanced nuclear reactors.

Office of Energy and Environment Initiatives: 505-667-3621 or http://www.lanl.gov/energy
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Yucca Mountain Project Radionuclide Transport

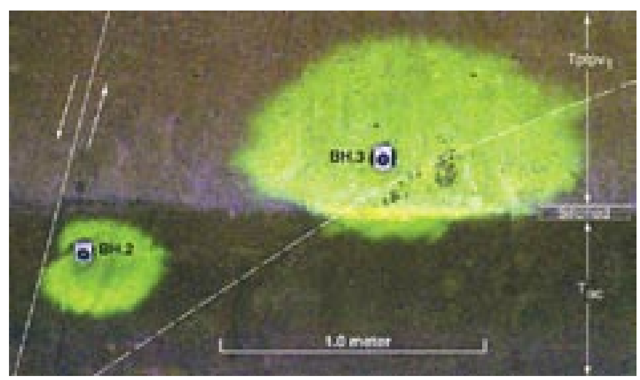
The Challenge: Ensuring Yucca Mountain Meets Waste Repository Requirements

Under stringent quality assurance procedures, Los Alamos has played a key role in preparing the programmatic documents used as the technical justification for the Department of Energy (DOE) to propose Yucca Mountain as the site of the first high-level radioactive waste repository. These documents represent the state of our scientific knowledge about the site and the potential for the geologic rock layers to retard the migration of radionuclides. The numerical models developed by Los Alamos were used directly in the performance assessment system model that was used to show that the Yucca Mountain site meets the regulatory requirements for a high-level radioactive waste repository.

Los Alamos Innovation: Characterizing the Hydrology and Geology Beneath Yucca Mountain

Moving forward represents the culmination of several decades of integrated research by Los Alamos scientists and collaborators on the hydrology and radionuclide transport characteristics of the geologic layers and the underlying aquifer beneath Yucca Mountain. Los Alamos has assembled an integrated program with laboratory experiments, field testing, and numerical modeling that has

- Characterized field samples;
- Measured the solubility and sorption of radionuclides;
- Studied transport rates in laboratory columns;
- Investigated the role of colloids in facilitating radionuclide transport;
- Performed hydrologic and tracer testing in the saturated and unsaturated zones;
- Calculated the conceptual model and determined model parameters;
- Assessed the groundwater system with hydrochemical sampling and data interpretation;
- Predicted radionuclide migration in the water table by modeling the unsaturated zone;
- Modeled flow and transport in the saturated zone to understand the hydrology, integrate the field data, and predict radionuclide transport; and
- Designed small-scale models of specific field tracer tests to understand the transport mechanisms and determine parameters for large-scale models.



The Impact: Removing Barriers to the Continued Use of Nuclear Energy

Based on Los Alamos's work, the Department of Energy was able to investigate all aspects of the issue, including engineering the underground facility, designing the manmade barriers, characterizing and predicting the migration of radionuclides in the geosphere, and isolating waste with the highest probability of public safety for acceptable time periods. The science performed in the Yucca Mountain project can not only renew progress in solving problems that have prevented the continued and expanded use of nuclear energy, but it also can be applied to other environmental water quality projects.

Office of Energy and Environment Initiatives: 505-667-3621 or http://www.lanl.gov/energy
Los Alamos National Laboratory is operated by the University of California for the U.S. Department of Energy.
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Space Reactors

The Challenge: Safe and Reliable Space Power and Propulsion

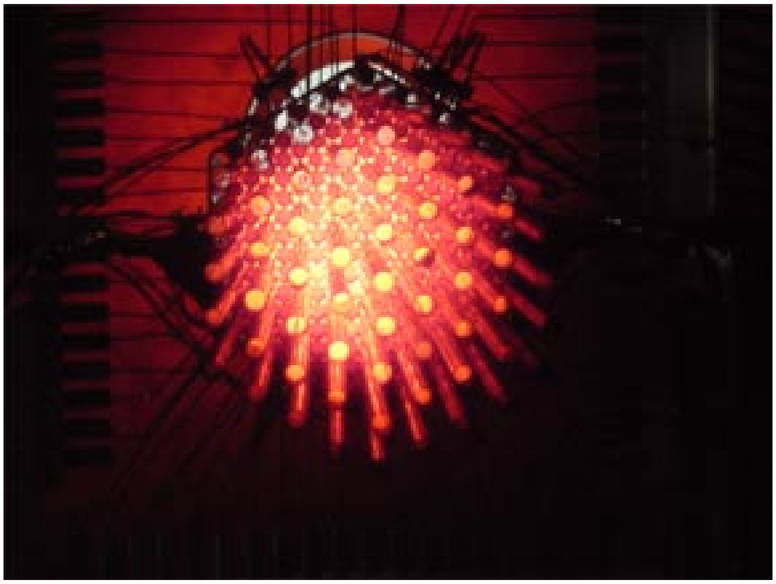
Los Alamos began a low-level effort in the mid-1990's to rejuvenate interest in space fission power and propulsion systems. The focus of the Laboratory's approach was on simple, highly testable systems that could enable space missions.

Los Alamos Innovation: Highly Testable Space Reactor Designs

In 1998, Los Alamos began working closely with NASA to design and fabricate potential space fission power reactor cores (unfueled), with a particular emphasis on testability. In 2000, realistic testing of one such core was initiated, with resistance heaters used to closely mimic fission heat deposition. In 2001, the core was coupled to a power conversion subsystem and an ion thruster to provide an end-to-end nuclear electric propulsion breadboard. Also in 2001, NASA began expressing interest in the development of space fission systems. The Los Alamos-led team continues to perform design, analysis, and testing related to a variety of space reactor concepts. Los Alamos is currently the reactor design lead for NASA's Jupiter Icy Moons Orbiter (JIMO) Project.

The Los Alamos-led team continues to demonstrate that innovative, highly testable space fission systems can be devised to enable numerous missions. The proposed designs facilitate conversion of paper reactor designs into actual working hardware. Designs emphasize test effectiveness (i.e., the ability to complete highly realistic non-nuclear testing). Systems are designed to be resistant to radiation damage and to have modest fuel burnup requirements, further increasing the worth of realistic non-nuclear testing. Numerous hardware tests have been performed to confirm the potential performance of the proposed systems.

SAFE-100 core simulator test performed during development of a reactor for NASA's Jupiter Icy Moons Orbiter (JIMO).



The Impact: Space Missions Requiring High Power Where Solar Power is Not Available

Space fission power and propulsion systems could enable numerous exciting space missions. Space fission systems are especially attractive for space missions requiring high power and/or missions operating in environments where solar power is not readily accessible. Potential missions include long-duration travel to the lunar or Martian surface and NASA's Jupiter Icy Moons Orbiter.

Spent Fuel Treatment

The Challenge: Reducing the Life Span of Spent Fuel and Recovering Energy Value

A nuclear power plant generates electricity using the energy released from the fission of certain isotopes present in the fuel, mainly uranium-235 and plutonium-239. The fission process produces many radioactive fission product elements. As the fuel is consumed in the reactor to release energy, the reduction in the amount of fissile isotopes in the fuel, and the build-up of fission products that absorb neutrons, makes replacement of some of the fuel elements necessary. Because radioactive decay produces heat, the spent fuel is removed from the reactor and stored underwater to cool. The spent fuel contains substantial amounts of energy in the remaining fissile elements and the "ashes" or fission products from the "burning" of the nuclear fuel. In the once-through fuel cycle, the spent fuel is allowed to decay for decades, until it is easier to package it in a container for final disposal in an underground repository. The repository must be capable of retaining some of the radioactive elements in the spent fuel, such as plutonium and technetium, for hundreds of thousands of years.

The goal is to separate the spent fuel into packages, thereby reducing life span and recovering energy value. The challenge is to accomplish this economically, safely, and with advanced operational safeguards. The current technologies used to treat fuel in France, the United Kingdom, Japan, and Russia recover uranium and plutonium from the fuel for recycle. However, the costs are high and improved separation of the fission products and other actinide elements is needed to optimize the overall fuel cycle and increase proliferation resistance.

Los Alamos Innovation: Revolutionary Separation Approaches

The work at Los Alamos on spent fuel treatment processes ranges from evolutionary to revolutionary. This includes developing a crystallization process based on standard industrial methods for recovering uranium, neptunium, and plutonium from spent fuel that has been dissolved in nitric acid and evaluating a revolutionary approach to separating actinides from the fission products in spent fuel based on aqueous carbonate solutions. Los Alamos's innovations have also allowed for the exploration of actinide and fission product separations in ionic liquid solutions and the exploration of high-temperature methods to reduce the cost of decladding the spent fuel and to remove selected fission products from the fuel. The Laboratory has also been developing selective and energy-efficient membrane-based separation systems as well as new nuclear fuel structures to simplify the recovery of the actinides from the fission products after the fuel is used.

The Impact: Recycling Spent Fuel and Reducing Waste

New technology is under development at Los Alamos to recover the energy value and more effectively manage the fission products. These technologies separate the components of spent fuel to recycle actinide materials for further use in power production while packaging the fission products more efficiently for disposal, transmutation, or other uses. The result would greatly increase the amount of waste the repository can accept, and the waste will decay to levels similar to those of natural uranium ores in a few hundred years.

A loop crystallization apparatus being tested to form crystals of uranium (VI) nitrate in a continuous process. The crystallization method could provide a more cost effective way to separate uranium from a solution of spent fuel dissolved in nitric acid.

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Physics Code Development

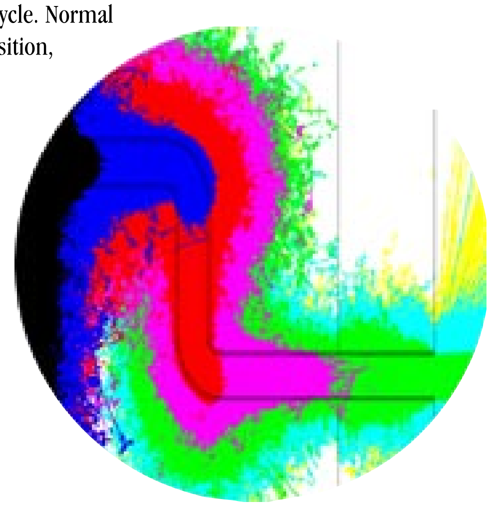
The Challenge: Creating Accurate Radiation Transport Computer Simulations

Accurate radiation transport computer simulations are fundamental in the design and operation of nuclear facilities. Such codes are important for reactor design, criticality determination, shielding design, dosimetry and heating calculations, and safety parameters estimation. Isotopic burnup simulation is key for waste transmutation, but capture and decay data must be modeled for thousands of isotopes in ground and metastable states. Therefore, the computer code must accurately simulate reactor geometry, particle flux, and changing elemental fuel composition at varied temperatures.

Los Alamos Innovation: MCNPX and CINDER'90 Codes

An experienced team of researchers is using the Monte Carlo radiation transport simulation approach, including both the MCNPX (3-D Monte Carlo) and the CINDER'90 (burnup) codes. The MCNPX code simulates the tracking and interactions of all particles over a wide range of energies and uses standard evaluated nuclear data libraries or in-line models when libraries are lacking. While building upon Los Alamos's work in Monte Carlo simulations, dating back to the Manhattan Project era, new techniques are being developed to increase simulatioin accuracy. The CINDER'90 code tracks nuclide evolution in a system when subjected to a pre-determined periodic neutron flux and is now being adapted to handle proton flux. Preliminary coupling was first enabled with the Monteburns code, and Los Alamos now seeks to fully integrate the two into a new package. Enabling a continually changing material description in MCNPX through the addition of the CINDER'90 burnup routines will give an accurate picture of material evolution through the entire reactor run cycle. Normal MCNPX tallies also enable the calculation of all standard parameters such as criticality, energy deposition, and particle flux at any point in the run cycle.

Example calculation showing neutron streaming through a waveguide penetration in a high-power industrial accelerator.



The Impact: A Wide Range of Applications

The MCNPX project has over 1,100 users from more than 250 U.S. and international institutions. Applications include

- Reactor and accelerator-based transmutation,
- Design of nuclear propulsion reactors for space missions,
- Neutron scattering experiments at spallation targets,
- Reactor and accelerator health physics,
- Medical applications (proton, photon, electron, and neutron therapy),
- Oil well logging,
- Irradiation facilities design and analysis,
- Radioisotope production,
- Neutral and charged particle radiography, and
- Detectors and experiments for nonproliferation and homeland defense.

Nuclear facility design relies upon radiation transport simulation, and Los Alamos's codes already ensure safe operation for existing installations. Recent notable uses for the Los Alamos code include

- Calculations of accurate radiotherapy doses delivered to patients with tumors,
- Verification of water on Mars, as published in *Science* (July, 2002), and
- Design of the Oak Ridge Spallation Neutron Source target and shielding.

This project also includes the development of parameter calculations for externally driven criticality sources and the pursuit of new variance reduction, tallying, and error analysis techniques.

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Thermal-Hydraulic System Code Development and Applications

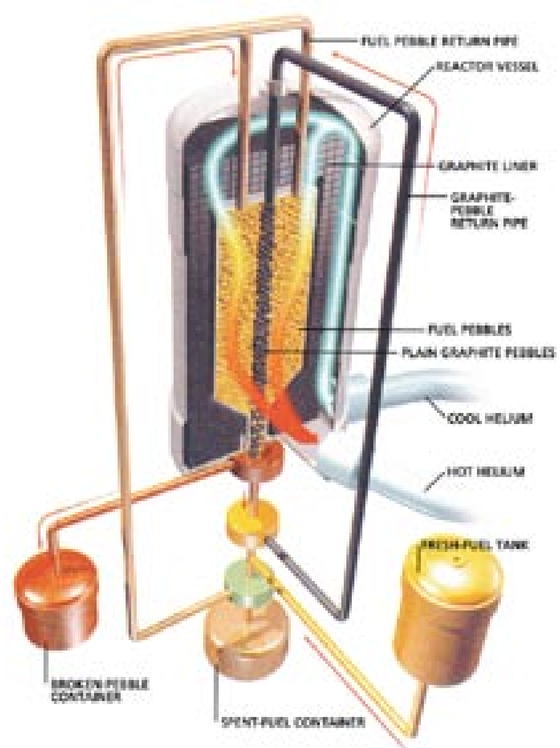
The Challenge: Modeling Nuclear Reactor Safety

In order to assure the safety of nuclear reactors, independent safety analyses are performed using best-estimate thermal-hydraulic codes. The TRAC/RELAP Advanced Computational Engine (TRACE) code, being developed by Los Alamos and other institutions for the U.S. Nuclear Regulatory Commission (NRC), has been used to model nuclear power plants and simulate accident scenarios to show that safety systems can bring the plant to safe shutdown conditions.

Los Alamos Innovation: The TRAC/RELAP Advanced Computational Engine

The TRAC/RELAP Advanced Computational Engine has been under continuous development by Los Alamos for the NRC since 1970. The TRACE code continues to evolve with increasing understanding of complex 2-phase, multi-component fluid phenomenology. After sponsoring multiple codes for over 2 decades, the NRC has selected TRACE as the sole platform for future development. Los Alamos plays a key role in an ambitious multi-institution development program to modernize and expand the existing code capabilities. As the NRC considers pre-application review of new reactor concepts such as the Pebble Bed Modular Reactor and the Simplified Boiling Water Reactor, Los Alamos is in a position to provide developmental and analytical support. Laboratory expertise is further leveraged by code development support for the Knolls Atomic Power Laboratory (KAPL), which has chosen TRACE as their best-estimate code.

Illustration of an advanced GEN-IV pebble bed modular reactor.



The Impact: Safer Nuclear Power Plants and Facilities

In support of the Accelerator Transmutation of Waste program, TRACE has been updated to include liquid-metal fluid properties and to enable the tracking of trace species. A TRACE model of the Los Alamos DELTA loop facility, a liquid lead-bismuth materials test loop, has been developed and used to simulate actual test runs. Recent TRACE code development tasks have sought to provide new Pebble-Bed core, materials, and component models, as well as revised channel modeling for the simplified boiling water reactor. Enhancements include three-dimensional fuel sphere-coolant heat transfer capabilities for the pebble bed modular reactor, and modeling capabilities for the water rods and partial-length fuel rods associated with the advanced boiling water reactor fuel designs. Additional implicit heat structure development support for KAPL will reduce run-times on key design basis accident analyses. In the future, Los Alamos scientists look toward developmental tasks in support of the GEN-IV reactor concepts, as well as the potential for hybrid code development, coupling TRACE to computational fluid dynamic and/or reactor physics analysis kernels.

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Assessing the Vulnerability of Nuclear Installations

The Challenge: Understanding Nuclear Facility Vulnerabilities and their Consequences

Los Alamos National Laboratory has been working with the Department of Energy, the Nuclear Regulatory Commission, and Sandia National Laboratories to support the development of a robust methodology to analyze potential threats to nuclear installations. This effort has led to capabilities and tools for a flexible approach to vulnerability assessment (VA) based upon the threat to a facility. Los Alamos is capable of providing the following information in support of facility VA's:

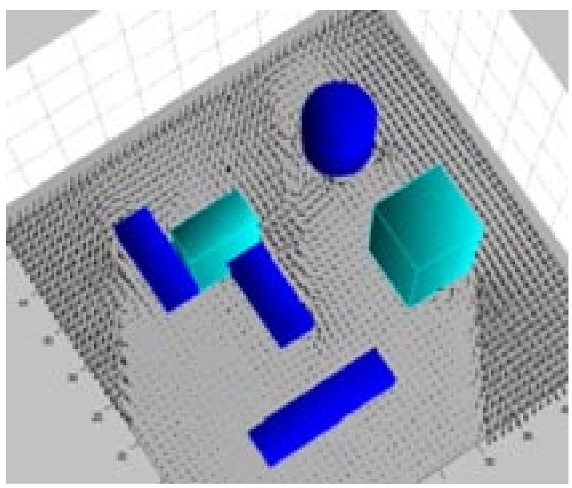
- Identification of threat sources, threat attributes, and potential targets;
- Identification of possible attack scenarios, including assessment of likelihood and consequences;
- Evaluation of existing protection and benefits of identified improvements.

Los Alamos Innovation: Using Probablistic Risk Assessment and Other Analysis Tools

The same technologies used in assessing postulated nuclear facility accidents and their consequences can be applied to postulated terrorist attacks on those same facilities. These technologies include

- **Probablistic Risk Assessment (PRA)—**Risk is a metric for comparing attack scenarios, requiring estimates of the probability of occurrence as well as conditional probability of consequences given the attempt. The primary tool for evaluating risk is the Logic Evolved Decision tool, which uses logic models and approximate reasoning to produce estimates of attempt probability through qualitative and subjective inputs.
- **Interior Aerosol Transport Modeling—**Calculation of aerosol transport in buildings is fundamental to most nuclear safety issues. Los Alamos uses many tools to estimate the transport of aerosol particles through a building and its ductwork to the environment. These tools range from simple calculations to complex 3-D flow codes.
- **Atmospheric Dispersion Modeling—**Atmospheric dispersion is the key transport mechanism for the release of most hazardous materials, including nuclear materials. Los Alamos utilizes industry standard and in-house tools to evaluate atmospheric dispersion. Tools include the Los Alamos-modified INPUFF code and the Los Alamos QWIC-URB and HIGRAD codes. The INPUFF code utilizes a Gaussian puff model for computational efficiency. At the other extreme, HIGRAD resolves 3-D flow field effects with realistic meteorology (near-field atmospheric dispersion). QWIC-URB provides an intermediate approach that employs empirically based multi-dimensional effects in the building wake regions, yielding improved accuracy over the far-field approach without the computational penalty associated with a full computational fluid dynamics analysis.

A QUIC-URB computer simulation of the air flow around a group of buildings. Wind vectors from one of the horizontal planes are shown. Note the steering of the wind, reverse flow, and pockets of calm air that develop downwind of the buildings.



The Impact: Secure Nuclear Facilities

Los Alamos National Laboratory's vulnerability assessment tools will help keep the nation's nuclear facilities safe and secure from accidents or potential terrorist threats.

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Nuclear Cross Section Measurements

The Challenge: Transmuting Nuclear Waste

Radioactive waste may be destroyed through neutron absorption, but the rate of destruction depends on the material's propensity to absorb neutrons, or "cross section." Isotopes with high absorption cross sections transmute more readily in systems with high neutron populations. While cross sections of commonly used isotopes in conventional nuclear fuel are well known, they are less well known for isotopes of neptunium, americium, and curium, as well as some isotopes of plutonium. In turn, there is uncertainty in the performance of proposed transmutation systems, whether they are reactor-based or accelerator-driven. The work that Los Alamos is doing in measuring cross sections of major spent nuclear fuel constituents will reduce the uncertainty of the proposed transmutation system's performance and add confidence to the selection process.

Los Alamos Innovation: Applying Unique Expertise and Instrumentation

The Los Alamos Neutron Science Center is without match for producing neutrons with kinetic energies from millielectron volts to hundreds of megaelectron volts with an array of detection systems unparalleled in the world. Los Alamos already has the instruments necessary to overcome obstacles, such as background from radioactive decay of the isotope. These instruments include

- **DANCE**—measures neutron capture cross sections;
- **GEANIE**—detects gamma rays emitted after neutron capture, giving insight into the nuclear structure of compound nuclei, and can be used to measure the inelastic scattering cross section of some isotopes; and
- **FIGARO**—measures higher-energy fission cross-sections and gamma rays emitted by neutron-induced nuclear reactions, and it detects secondary neutrons emitted by these reactions.

Los Alamos has the expertise in fabricating and handling the actinide targets necessary for these measurements.

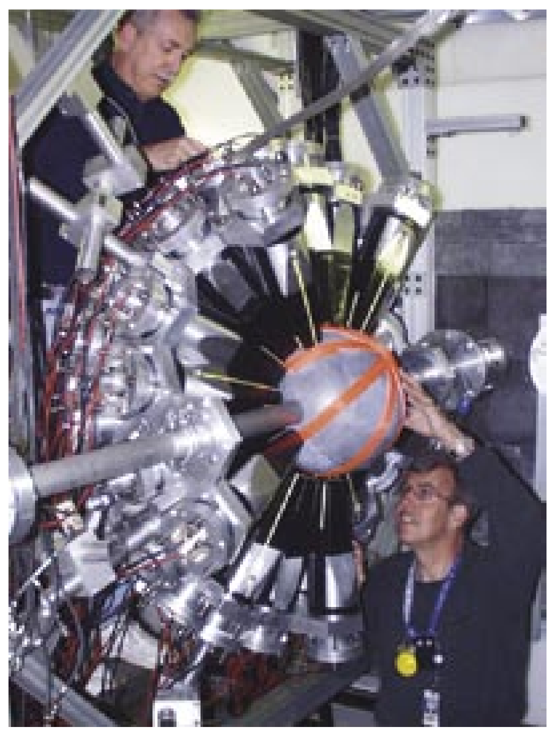
The Impact: Assessing Transmutation System Performance

Los Alamos's effort to measure the capture and fission cross sections of the minor actinides involves

- Fabrication of radioactive samples;
- Preparation of safety documentation;
- Acquisition of data from experiments;
- Analysis of experimental data; and
- Publication of the results.

This effort is a natural fit with other Los Alamos capabilities, especially those of the Nuclear Data and Theory group which will aid in choosing the cross sections to be measured. They are the primary users of the experimental results that will ultimately be obtained. Researchers in the Systems Engineering and Integration group, and worldwide, will use the developed and evaluated nuclear data to assess the performance of proposed transmutation systems.

The newly commissioned DANCE detector. The radioisotope whose capture cross section is to be measured is placed in the center of the red-taped spherical sample chamber. Gamma rays emitted as a result of neutron capture in this sample are detected in the barium fluoride scintillators that completely surround the sphere (a so-called "4π detector geometry"). In this photograph, half of the scintillators are moved away to allow access to the sample chamber.



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Coolant Technology for Nuclear Systems

The Challenge: Enhancing Safety and Reliability in Nuclear Coolant Technology

Nuclear coolant technology is considered to be one of the most critical and challenging issues in developing advanced nuclear systems, as can be seen in the Accelerator Transmutation of Waste (ATW) and Gen IV roadmaps. Safe and reliable nuclear coolant technology is a necessity. Mitigating safety issues of chemically active coolants, lead, lead-bismuth eutectic (LBE), and lead alloys—used as liquid metal coolants—represent a promising option in the liquid metal cooled waste transmuters and advanced reactors. Lead alloys are also potential target materials and coolants for high-power spallation neutron targets with multiple applications in accelerator-driven systems (ADS) and materials irradiation test facilities. This project targets the technology gaps for programmatic applications identified through analyses of the current state of the Lead-Bismuth Eutectic (LBE) technology, which is based on the Russian LBE nuclear coolant technology and the international ADS LBE technology development.

Los Alamos Innovation: Developing Lead-Alloy Coolant Technology and Materials

Los Alamos boasts a suite of research & development tools to

- Develop, calibrate, and test oxygen sensors;
- Characterize protective oxide films on steels and their irradiation behaviors;
- Model system corrosion kinetics in oxygen-controlled liquid metal systems;
- Develop active corrosion probes; and
- Adapt reactor safety code for systems cooled by lead alloys.

Among the unique test facilities and technologies at the Laboratory's disposal, Los Alamos's DELTA LBE test Loop is the only one of its kind in the United States, and one of very few outside of Russia. A medium-scale forced circulation LBE loop for materials and thermal hydraulics testing, the DELTA Loop allows for simultaneous testing of large arrays of materials by featuring

- Sophisticated design and engineering,
- Versatile instrumentation and control, and
- Implementation of coolant chemistry control.

The Impact: Reducing Risk and Producing Hydrogen

Coolant technology development is leading to other programs, which include

- Assisting AFCI and Gen IV in selecting technological options with reduced risks;
- Expert presence in Gen IV road mapping ensures lead-alloys-cooled fast reactors are properly evaluated and selected as one of six systems for further development;
- Capability to support the choice of lead-alloy-cooled systems for small, modular, deployable reactors; and
- Wider application of test facilities, materials, sensors, instrumentation, and control techniques developed for nuclear coolant.

Using liquid metal as a reforming medium may lead to alternative hydrogen production processes with reduced greenhouse gas emissions and automatic carbon sequestration, supporting the national hydrogen initiative and emphasizing nuclear and solar productions.

The DELTA Loop Test Facility including support, enclosure, and access structures. The data acquisition and control console are in front of the enclosed loop experimental apparatus. The DELTA Loop has been used in continuous corrosion test campaigns since the early part of 2003.

Magnetized Target Fusion

The Challenge: Developing Clean, New Energy Sources

The field of fusion energy research has been an endeavor of the U.S. government for nearly half a century. In the 1950's, through the efforts of Dr. Jim Tuck and "Project Sherwood," Los Alamos National Laboratory became controlled fusion's birthplace (ahead of Princeton by about 1 year). From the 1970's-1990, this research was carried on through the Controlled Thermonuclear Research (CTR) Division, and it continues today at modest levels in the Physics, Theory, and Chemistry Divisions.

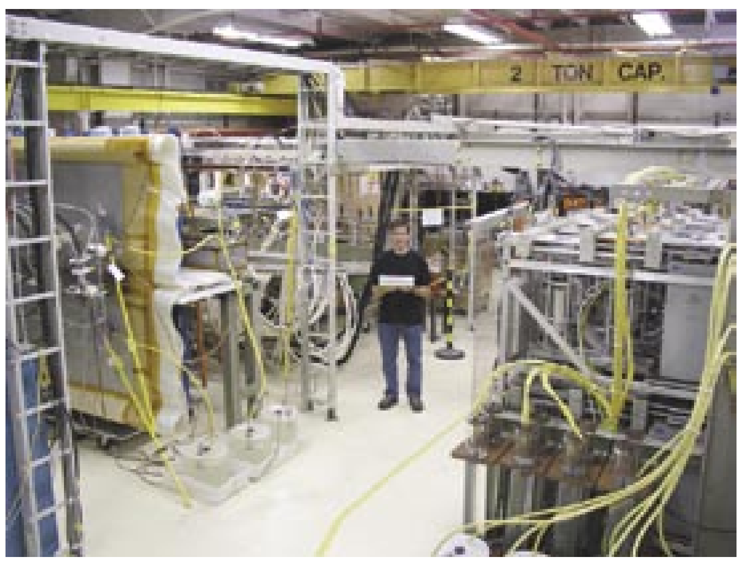
Los Alamos Innovation: Magnetized Target Fusion

In the Physics Division, Los Alamos is pursuing a radical approach to achieving a hot fusion plasma in the laboratory through "magnetized target fusion" (MTF), involving ideas from traditional magnetic fusion confinement and inertial fusion confinement. Magnetized Target Fusion involves forming a moderately warm, moderately dense hydrogenic plasma. Los Alamos proposes stuffing this "target plasma" into an aluminum can, which is quickly compressed by an electric current running down the can's walls. The resulting electromagnetic "J x B" force crushes the can in a precise, controlled fashion. Los Alamos and the Air Force Research Laboratory (AFRL) in Albuquerque have can-crushing pulsed power machines developed for defense programs testing. With 20 years of experience with compact toroid fusion plasma combined with current advances made in liner technology, Los Alamos and the AFRL hope to make the first physics demonstration of magnetized target fusion within 4 to 5 years.

The Impact: A New Energy Alternative for the Future

Fusion energy research is a challenging, multi-faceted project requiring the efforts of many scientists and engineers in collaboration throughout the world. Los Alamos aims to produce fusion-grade plasma quickly and cost effectively by mostly using existing facilities. A long-term vision for the MTF project is for the creation of a liquid-walled fusion reactor based on the MTF principles. This reactor would give a pulse of fusion energy every 10 seconds, with a new liner dropped into place between pulses and new target plasma injected into the liner. Before such a reactor could be realized, significant advancements must first be achieved in materials, sensors, controls, and engineering.

With the severity of long-term energy needs, persistence is key. Nuclear energy is split into fission and fusion energy. Fission reactors already produce significant electrical power to the grid, while fusion researchers can only talk about a 35-year plan to demonstrate the first power producing fusion reactor demo. Success in a project like MTF, offering an "orthogonal" approach to achieving fusion quicker and cheaper, would be a first step toward making a fusion reactor quite differently than presently planned by the scientific community.



FRX-L plasma injector experiment at Los Alamos National Laboratory. A researcher holds an aluminum liner.

Future Directions

A Nuclear-Powered Future and the Role of the United States

A reliable energy supply is vital to modern civilization. The availability of unfailing energy sources underpins our national security, economic prosperity, and global stability. There are signs, however, that our current energy supply is not reliable. Our world may soon see unprecedented new demands for energy leading to resource depletion, conflict, and increased pollution. As one of the world's most powerful and prosperous nations, the U.S. must accept its role in developing a diverse energy supply system that meets rapidly growing world energy needs while promoting peace, prosperity, and environmental quality. Experience and independent studies tell us that no single resource will meet all our future energy needs in an economically and environmentally acceptable way.

Los Alamos National Laboratory Nuclear Program Goals

Despite the social stigma, nuclear energy has much to offer. Today, the 103 nuclear power plants operating in the U.S. produce more than 20 percent of the nation's electricity. The average plant operating costs for nuclear power are less than for coal, and about one-third of those for natural gas. Nuclear-generated electricity produces none of the greenhouse gases and smog-producing chemicals released when coal and natural gas are burned, and nuclear fuel supplies are abundant and secure. Resuming U.S. nuclear advancements, nuclear energy could

- Become an energy source for producing hydrogen necessary to realize a zero emissions transportation system;
- Reduce the United States' CO_2 emissions by more than 3 billion tons per year, halving the emissions currently produced by electricity generation;
- Replace 2 billion barrels of imported oil per year with nuclear-generated hydrogen (the U.S. imports about 3.5 billion barrels per year);
- Enhance our nation's energy security;
- Make up half the U.S. electricity and a quarter of the hydrogen for transportation;
- Reduce long-lived nuclear waste by more than 98 percent; and
- Reduce the risk of nuclear materials getting diverted to weapons use.

Los Alamos National Laboratory Capabilities

Congress approved Yucca Mountain, Nevada as the used nuclear fuel repository. While a significant step, the current rate of waste production would require a repository the size of Yucca Mountain every 30 years (every 15 years if nuclear energy grows at 1.5 percent per year). The Nuclear Waste Policy Act directs the Secretary of Energy to decide on a second repository between 2007 and 2010. Providing an alternative solution to subsequent repositories, the Advanced Fuel Cycle Initiative (AFCI) proposes the recycling of used nuclear fuel, reducing the long-lived nuclear waste and capturing the remaining energy potential. Over 96 percent of spent nuclear fuel is uranium, the remainder being fission products, plutonium, and higher actinides. The AFCI's plan is to reuse the uranium, allowing short-lived fission products to decay, recycle, and transmute the plutonium and higher actinides. This greatly reduces the opportunity for diversion or misuse of nuclear materials because they are destroyed and not stored for millennia. This spent fuel treatment eliminates the need for additional repositories and reduces the risk of nuclear proliferation. These advanced technologies, combined with advanced techniques for transparent material accountability, will set future world standards for nuclear proliferation prevention and global nuclear materials management.

WATER

Energy and Environment Compendium

Los Alamos
NATIONAL LABORATORY

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Water Research at Los Alamos National Laboratory

Water Research at Los Alamos National Laboratory

Water resource management has become a critical issue worldwide, the result of dwindling potable water supplies and expanding populations into regions with limited water reserves. In the United States, it is critical for national security and a strong economy that we ensure safe, dependable water supplies can meet the country's changing population demographics. Through its research in atmospheric, surface, and subsurface water, Los Alamos National Laboratory has conducted focused efforts to resolve risks and problems associated with water resources. The Laboratory has also guided technology developments to ensure dependable water resources and to protect human health and the environment.

With a cohesive strategy, the Los Alamos team pursues water research on multiple scales, from atoms to oceans, and across a broad range of issues, from ensuring clean, adequate water supplies to assessing water security risks and understanding the effects of societal shifts on water demands.

Current Scientific Challenges in Water Research

Creating integrated models based on acquired data is necessary to gain insight into water resource issues and to assist with trend prediction. Predictive decision analysis techniques can help decision makers analyze uncertainties, predict scenarios, understand trade-offs, and implement optimized solutions. Applying research results to real-world situations to protect and conserve our water resources, and educating both policymakers and the general public about water issues are the final goals of Los Alamos's water research programs.

Problem-Solving Capabilities in Water Research

- **Modeling and Simulation—**Los Alamos has expertise in modeling water on all scales, from models of atomic and molecular interactions to coupled models of river basins to integrated models of ocean currents and ice flow patterns.
- **High-Performance Computing—**Los Alamos researchers have high-performance computing facilities to execute complex simulations.
- **Observational and Experimental Methods—**The Laboratory has extraordinarily sophisticated observational and experimental methods, and has gathered data on atmospheric water, sediment, surface water, and groundwater.
- **Analytical Chemistry—**Los Alamos has the analytical chemistry expertise to solve key water quality issues.
- **Multidisciplinary Approaches to Complex Systems—**Exceptionally diverse multidisciplinary teams solve scientific and engineering challenges.
- **Data Management and Analysis—**Legacy databases are valuable resources to water quantity, quality, and interaction research.
- **Pollution Prevention—**Scientists and engineers at Los Alamos National Laboratory have long been involved in green chemistry activities and experiments involving various chemical and radioactive species, allowing them to develop expertise in minimizing the impact of these species on the environment.
- **Decision Analysis—**Procedures developed by the Laboratory to support military and national security decisions can be applied to help researchers and policymakers make more informed decisions regarding water issues.
- **Security and Threat Analysis—**The Los Alamos team has decades of experience in national and international nuclear security that can be applied to protect the civilian water supply.

Office of Energy and Environment Initiatives: 505-667-3621 or http://www.lanl.gov/energy
Los Alamos National Laboratory is operated by the University of California for the U.S. Department of Energy.
LALP-04-026

Española Basin Aquifer Model

The Challenge: Sustaining Groundwater Quantity and Quality

Maintaining a dependable and high-quality water supply in arid and semi-arid regions is a growing national concern, particularly because of prolonged drought conditions. In New Mexico, where groundwater provides more than 80 percent of public water supplies, Los Alamos National Laboratory and the surrounding area (Los Alamos, Española, Santa Fe, and many pueblos) rely on the Española Basin Aquifer. Declining water levels in the basin are of great importance to the Laboratory because of the implications for a sustainable water supply and because of the potential decline in groundwater quality.

Los Alamos Innovation: Large-Scale Yet Detailed 3-D Models

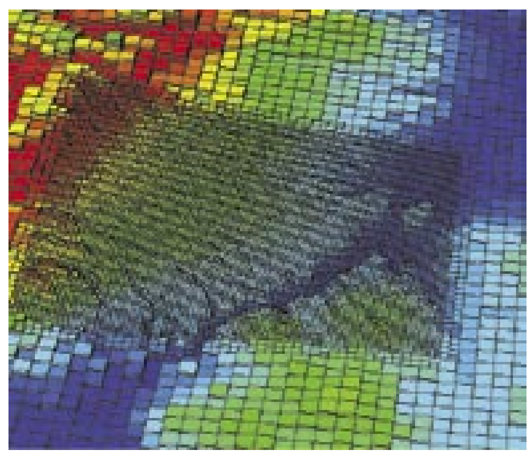
With an on-site technical team of geologists, geophysicists, geochemists, and hydrologists, Los Alamos is developing a unique, multidisciplinary approach to address basin-scale hydrologic questions, such as:

- How much high-quality water is in storage in the regional aquifer and how rapidly is this reservoir being depleted?
- What impact do aquifer withdrawals have on surface water flow?
- How will the drought affect groundwater supplies?

Answering these questions requires a simulation model that is sufficiently large in scale to encompasses the entire aquifer (approximately 100 square kilometers) but also sufficiently detailed to capture small-scale variations in hydrostratigraphy and stresses on the aquifer because of pumping. The high-performance computing facilities and flow and transport codes at Los Alamos provide a cornerstone for developing models with high resolution and tight coupling between hydrologic and geochemical processes. Using these tools, a large body of geologic, geophysical, and geochemical data has been integrated into a sophisticated 3-D model of the basin aquifer. Los Alamos has also developed and applied statistical methodologies for applying model predictions in decision-making contexts. The modeling and analysis tools can

- Predict the rate of future water level declines due to pumping;
- Predict the ultimate fate of contaminants in the regional aquifer;
- Optimize data collection in deep boreholes being drilled at the Los Alamos site;
- Evaluate the adequacy of groundwater monitoring strategies;
- Estimate the uncertainty of model predictions; and
- Visualize flow paths and aquifer characteristics in 3-D.

Close-up image of White Rock Canyon within the Española Basin numerical grid.



The Impact: Better Resource Management Locally and Beyond

Detailed analysis of these problems is important not only for the study area, but also regionally and globally. Benefits of the modeling include assisting Los Alamos National Laboratory and surrounding communities in evaluating potential threats to water quality and rates of aquifer depletion. The modeling and prediction methods developed for the Española Basin can be transferred to other regions to assist in widespread national and global resource management.

Los Alamos NATIONAL LABORATORY

Scanning Raman LIDAR

The Challenge: Accurate Measurement of Atmospheric Water Vapor

Many atmospheric greenhouse gases contribute to climate change, and the ones that have dramatically increased due to human industrial activity, such as CO_2, get most of the attention. But simple, common water vapor is probably the most important of all greenhouse gases. Water vapor's role as a greenhouse gas is little understood at present largely because of a lack of instrumentation that can "see" and measure its movement and fluctuations. However, Los Alamos National Laboratory is addressing this problem with its scanning Raman LIDAR—an ideal tool for measuring eco-physiological parameters in the atmosphere, including the fate and transport of water vapor over agricultural and forested sites.

Los Alamos Innovation: Using Laser Light for Selective Measurements

The U.S. Department of Defense requested that Los Alamos develop scanning LIDAR (Light Detection and Ranging) instruments to detect and monitor biological and chemical agents released into the atmosphere. Los Alamos built, tested, and fielded the scanning Raman LIDAR in an unprecedented 6 weeks. An outgrowth of this program is the scanning Raman water vapor LIDAR. LIDAR operates in a manner similar to radar. A beam of energy is bounced off a distant object and the reflected energy is measured. However, LIDAR uses laser light instead of radio waves to scan distant objects. Because molecules interact with light in very specific ways, different wavelengths can be used to detect very specific chemical compounds, so water vapor can be isolated from other atmospheric gases.

The Impact: Understanding the Water and Carbon Cycles

The Laboratory's ongoing LIDAR research will help explain the spatial distribution of water vapor and flux in the atmosphere boundary layer (the region extending 1 kilometer into the atmosphere) and produce a water vapor and flux mapping system at an extremely high resolution in space. Because water vapor is the most abundant greenhouse gas and an important part of the global hydrological cycle, LIDAR will play a critical role in understanding and managing the interdependent water and carbon cycles.

The mobile scanning day/night Raman water vapor LIDAR has operated on both terrestrial and ocean surfaces. The most recent efforts have been concentrated on open water evapotranspiration at Elephant Butte reservoir in southern New Mexico.

Los Alamos NATIONAL LABORATORY

Evapotranspiration Mapping and Riparian Consumptive Use

The Challenge: Addressing a Critical Unknown Variable of Riparian Vegetation Water Use

The Bureau of Reclamation (BOR) has identified riparian vegetation consumptive use of water, known as "evapotranspiration," as a critical unknown variable in understanding surface and subsurface water resources on watersheds such as the Rio Grande. Previous studies used point sensors to make evapotranspiration measurements, but uncertainty in the spatial variability precluded definitive results. To overcome this problem, the BOR in Albuquerque funded a water flux mapping study and requested Los Alamos participation. The ongoing research measures the water use of salt cedar and cottonwood—tree species common to riparian zones in the southwest—to determine if they differ in their water use. The goal is to improve water management on the Rio Grande.

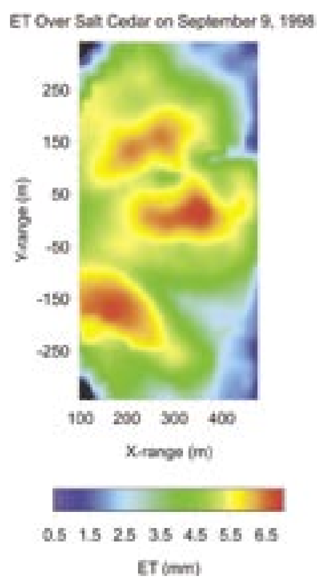
Los Alamos Innovation: Using LIDAR to Measure Evapotranspiration

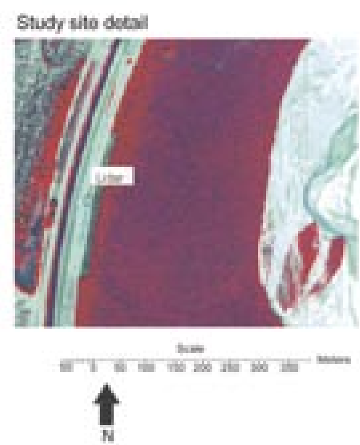
In coordination with universities in New Mexico and nationwide, the Laboratory has assembled an interdisciplinary measurement and analysis team to field, operate, and analyze data with its unique mobile scanning Raman water vapor LIDAR (Light Detection and Ranging) technology. LIDAR can measure evaporation thoroughly and accurately across time and space.

The Impact: Better Management of River Basins

The collaboration will help to better understand evapotranspiration at selected riparian sites along the Rio Grande and will result in the development of spatial maps of evapotranspiration over the Bosque del Apache study site to represent selected phonological periods in the riparian vegetation growth patterns. In addition, quantifying the spatial and temporal variability in evapotranspiration on local micro-scales will be possible as will the translation of spatial and temporal variability terms to an evapotranspiration model for sub-sections of the Rio Grande. The accurate measurement and modeling of this key variable will improve the management of river basins.

Using the scanning capability of the mobile Raman water vapor LIDAR, Los Alamos has developed a water vapor flux mapping system. The first image shows the spatial variability of evapotranspiration for a typical day in September over the salt cedars on the banks of the Rio Grande River; for reference, a false color infrared air photo of the site is shown at right.





Supercritical CO_2 Resist Removal (SCORR)

The Challege: Reducing Water Use in Integrated Circuit Manufacturing

An integral step in integrated circuit manufacturing is photolithography. This step requires large amounts of hazardous solvents and vast amounts of ultra-pure deionized water. Along with 100,000 gallons of solvents, a single fabrication plant may use up to 4 million gallons of water per day to ensure that all traces of organic solvents and sulfates are removed from the wafer surface. Ironically, many of the largest plants in this country are located in states already plagued with chronic water and occasional energy shortages: New Mexico, California, Texas, and Arizona. Responding to a technical request from Hewlett Packard (now Agilent Technology), Los Alamos began developing the Supercritical CO_2 Resist Removal (SCORR) technology to address this problem.

Los Alamos Innovation: Using Supercritical Carbon Dioxide as a Replacement Solvent

Los Alamos's SCORR technology has rapidly evolved to commercial implementation and meets performance goals outlined in the *International Technology Roadmap for Semiconductors*. As a replacement solvent for integrated circuit manufacturing, SCORR can

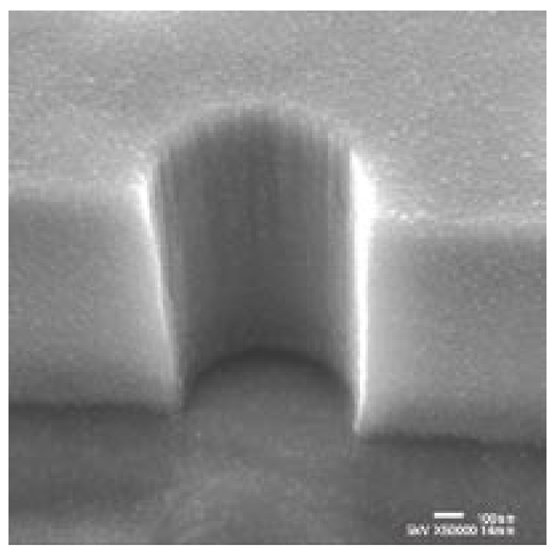
- Greatly reduce or eliminate the use of water;
- Eliminate energy requirements for drying wafers and purifying water; and
- Reduce, by 95 to 99 percent, the use of hazardous chemicals (chlorofluorocarbon compounds, hydrogen peroxide, sulfuric acid, acetone, methyl-ethyl ketone and isopropyl alcohol.)

SCORR is a technically-enabling green process that is not only accepted but driven by leading semiconductor and IC manufacturers as well as equipment and material suppliers.

Scanning electron microscopy of nano-sized structure before the residue from plasma etch processing has been removed (above) and after removal using the SCORR process (below).

The Impact: SCORR Will Enable Smaller Integrated Circuits and Other Nanotechnologies

To continue on their astounding growth curve, integrated circuits must become smaller, faster and cheaper. The *International Technology Roadmap for Semiconductors* details the technological barriers that must be overcome to fabricate integrated circuits with diminishing feature sizes. Because of their high viscosity, the traditional liquid solvents currently used will not be able to clean these small features. With SCORR, the smallest features present no barriers because supercritical fluids have zero surface tension and a gas-like viscosity, which allows them to remove particles smaller than 100 nanometers from integrated circuit features.



Los Alamos's developments in SCORR technology can enable industry to advance to increasingly finer architectures by removing a rate-limiting technical hurdle for the industry while cutting cost and nearly eliminating environmental liabilities. SCORR technology can also allow for the use of supercritical fluids to expand into many other fabrication processes and into other areas of nano-technology such as flat panel displays, Micro-Electro Mechanical (MEM) devices, and memory.

Los Alamos
NATIONAL LABORATORY

Plants with Improved Water Use Efficiency

The Challenge: Using Plants to Manage Atmospheric Carbon

Los Alamos has adopted a project to optimize the water efficiency of plants. This project is of special interest to two major U.S. industries: energy and agriculture. In addition to being the nation's largest users of water, the two industries are acutely interested in hardy, easily sustained plants for separate reasons. While agriculture has a keen financial interest in more water-efficient plants, the energy industry's particular interest is based on the role of plants in carbon sequestration. In the arid and semi-arid western United States, where precipitation is scarce, improving water efficiency is essential to using the natural ability of plants to capture CO_2 from greenhouse gas emissions.

Los Alamos Innovation: Enhancing the Water Use Efficiency of Plants

Los Alamos has developed and patented a unique approach to enhancing the water use efficiency of plants. Because well-nourished plants require less water, the Laboratory has focused on developing plants that take up and use nutrients more efficiently.

Using the Laboratory's strengths in DNA sequence-based techniques, in combination with isotope-assisted metabolic analysis, researchers developed the ability to manipulate plant growth by influencing the plant's own metabolic coordination of carbon and nitrogen. They were also able to characterize the nutrient-use systems of a set of experimental plant systems and develop a prototype plant with improved nitrogen use and water use efficiencies.

Engineered plants with increased growth and water use efficiency.

The Impact: More Efficient Crop Production and Control of Atmospheric Carbon

With results far beyond the original goals of the project and with the technical approaches applicable to both traditional and modern biotechnology, the generation of even more water-efficient plants is possible. These plants could serve as a valuable way to reduce CO_2 in the atmosphere and contribute to more water-efficient agricultural production.

ZeroNet Water

The Challenge: Increasing New Mexico's Power Without Increasing Water Usage

New Mexico has serious water problems that will be exacerbated by continued population growth and a potential long-term drought. The ZeroNet Water-Energy Initiative's goal is, by 2010, to meet New Mexico's increasing electric power demand without increasing water use for power plant cooling.

Los Alamos Innovation: Creating Multiple Options Through Multiple Partners

Los Alamos National Laboratory, The Electric Power Research Institute, and the Public Service Company of New Mexico (PNM) together have created ZeroNet. ZeroNet provides support tools to manage competition for water resources while accelerating current technological innovations. To further these initiatives, ZeroNet has pursued an aggressive technology transfer and implementation schedule.

Partners from industry, other national laboratories, universities, and state and federal governments ensure capabilities are leveraged to provide multiple water use solutions. ZeroNet takes a comprehensive and integrated approach by incorporating the following program elements:

- Degraded water use—alternative water sources for cooling systems;
- Integrated modeling and management scenario assessment—approaches include Watershed Analysis Risk Management Framework and Integrated Basin Model;
- Economic, market, and risk analysis;
- Water efficiency, conservation, recycling, and renewables;
- Monitoring and measurement;
- Advanced cooling; and
- Land management (piñon, juniper, and upland forest thinning, removal of non-native riparian species).

PNM's San Juan Generating Station near Farmington, N.M. will serve as a test site for the ZeroNet Initiative.

The Impact: Adequate Supplies of Electricity and Water for the Future

This initiative will deliver new electric power capacity in New Mexico with "zero net" freshwater withdrawals while ensuring a stable water resource for energy producers. Energy costs will be reduced because clean, affordable water can be provided. Los Alamos will also create a detailed source of water and energy information to aid the public and policy-makers and will provide targeted technological solutions and technology transfer opportunities. The quality of the nation's fresh water supply will be improved and competition between energy producers and other water users will be alleviated. The result will be an innovative model that can be adapted for other states and regions.

Los Alamos NATIONAL LABORATORY

Groundwater Remediation

The Challenge: Cleaning Up Groundwater Pollution

Groundwater is a precious resource in many regions, especially in arid places like New Mexico. After 50 years of serving the nation's defense needs, Los Alamos National Laboratory discovered that the alluvial (shallow) groundwater within nearby Mortandad Canyon had been contaminated with radionuclides, perchlorate, nitrate, and other inorganic chemicals. In response, Los Alamos developed the concept of multipermeable reactive barriers, which are designed to remove a variety of inorganic chemicals and radionuclides using natural materials. The materials were tested in the laboratory prior to designing the permeable reactive barrier (PRB) to be installed in Mortandad Canyon. The Mortandad Canyon field site was selected based on the nature and distribution of contaminants found in alluvial groundwater.

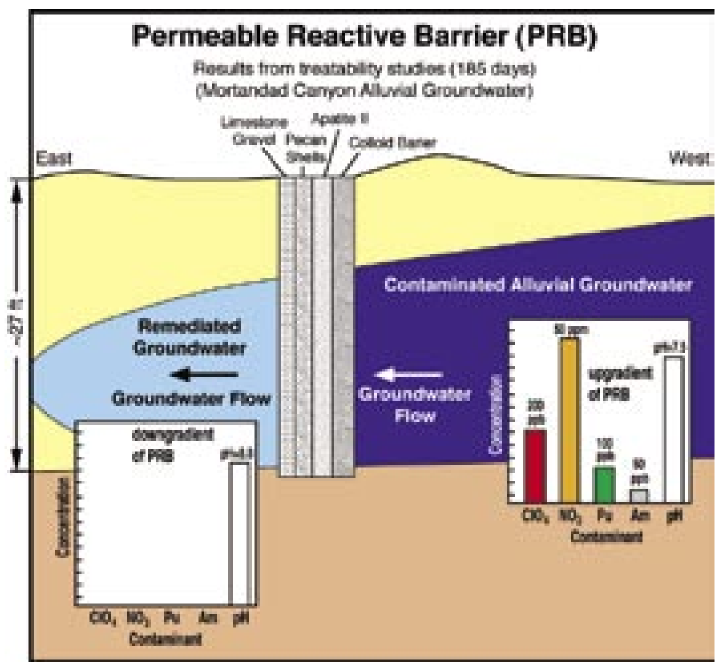
Los Alamos Innovation: Combining Natural Materials to Remove Inorganic Contaminants

A multidisciplinary team was selected to work on the PRB project, integrating Los Alamos's capabilities in hydrology, geochemistry, geology, engineering, regulatory compliance, and computer modeling. The PRB is a passive system that eliminates the need to pump and treat contaminated alluvial groundwater, which is costly and ineffective for most inorganic chemicals and radionuclides. It also removes contaminants through adsorption, biodegradation, and precipitation. It consists of natural materials (calcium hydroxylphosphate, cottonseed meal, pecan shells, and calcium carbonate) that achieve desired reactions with specific contaminants. As a result, radionuclides are removed by adsorbing onto calcium phosphate and coprecipitating with other metals and phosphate. Perchlorate is then biochemically reduced to chloride by cottonseed meal while nitrate is reduced to nitrogen gas under anaerobic conditions enhanced by cottonseed meal and carbonate, with a pH range between 7 and 8, neutralizing groundwater within the PRB.

The Impact: Safe Groundwater in Northern New Mexico and Beyond

Since alluvial groundwater migrates through the subsurface and impacts deeper groundwater within Mortandad Canyon, it is important to remove inorganic contaminants from alluvial groundwater within the canyon. Installing the PRB will help to remediate alluvial groundwater, including the regional aquifer, and reduce the volume of contaminated groundwater migrating through the subsurface. PRB technology can be applied at other sites contaminated with metals, perchlorate, nitrate, radionuclides, and other inorganic contaminants.

Schematic cross section of the multiple permeable reactive barriers installed in Mortandad canyon.



Los Alamos NATIONAL LABORATORY

Semi-Arid Hydrology and Riparian Areas

The Challenge: Maintaining Sufficient Water Resources in Semi-Arid Regions

In 2001, the National Science Foundation (NSF) Science and Technology Center for Sustainability of Semi-Arid Hydrology and Riparian Areas (SAHRA) began operations with a mission to promote sustainable management of water resources in semi-arid regions. Led by the University of Arizona, other participants include the University of New Mexico, New Mexico Tech, University of California Riverside, University of California Los Angeles, other universities, and government agencies. Los Alamos National Laboratory is a partner in the SAHRA multidisciplinary team and leads the effort in multi-resolution integrated modeling of basin-scale processes.

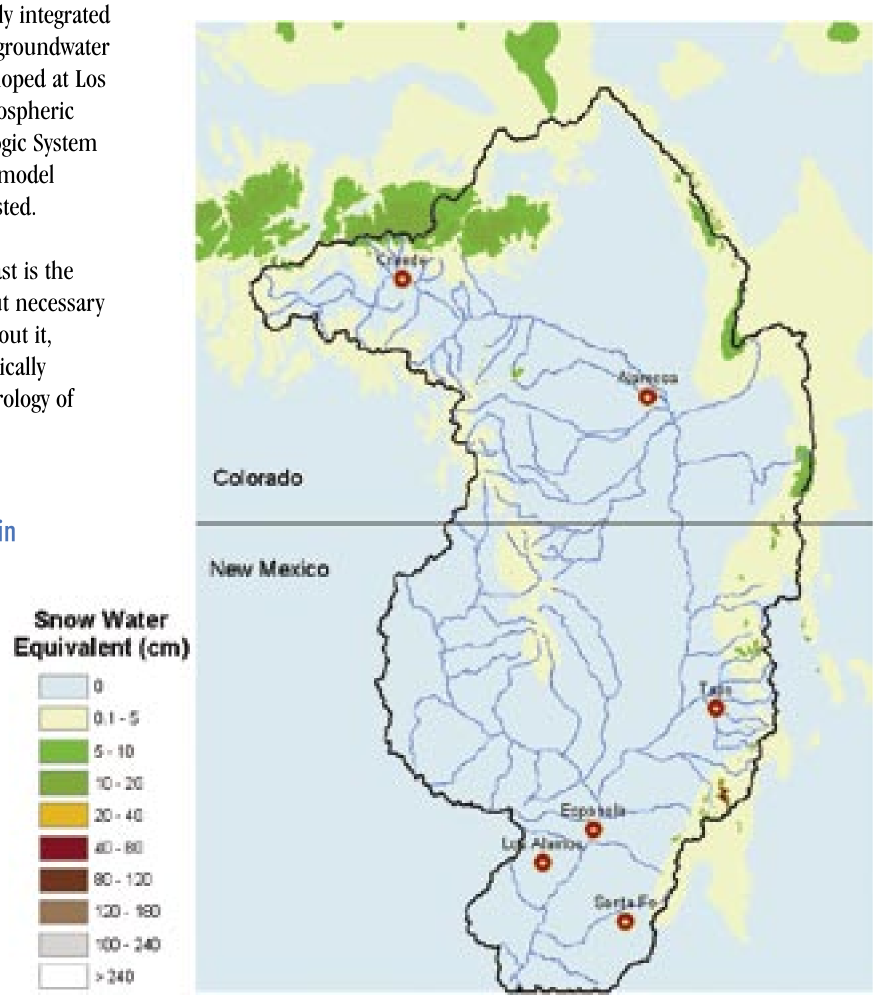
Los Alamos Innovation: Integrating High-Resolution Models

Los Alamos's unique capabilities in high-performance computing and modeling have resulted in the creation of an integrated, high-resolution model to understand and predict the effects of climate variability and land use change on the water balance. The Laboratory's participation in SAHRA has allowed for rapidly integrated computer codes that simulate atmosphere, surface, and groundwater components. The Parallel Applications Workspace—developed at Los Alamos—has also been used to couple the Regional Atmospheric Modeling System and the Los Alamos Distributed Hydrologic System with minimal changes to the two application codes. This model simulates the Rio Grande Basin, where it is now being tested.

One major interface that has not been exploited in the past is the socio-economic modules. This interface is challenging but necessary for models to be successful in supporting decisions. Without it, policymakers can fail to see the strong personal and politically sensitive reasons behind studying and protecting the hydrology of semi-arid riparian areas.

The Impact: Better Management of Water Resources in Semi-Arid Regions

Los Alamos's participation in SAHRA has provided the Laboratory with an opportunity to apply its expertise to critical water resource problems in New Mexico and the southwestern United States.



Simulated distribution of snow water equivalent across the Rio Grande Basin above Cochiti Reservoir.

Hydrogeologic Model of the Pajarito Plateau

The Challenge: Collecting Data on the Pajarito Plateau Aquifer

Los Alamos National Laboratory is located on the Pajarito Plateau in northern New Mexico. Research on the hydrogeology of the Pajarito Plateau began as an outgrowth of the Rio Grande Project and the implementation of the Hydrogeologic Workplan for the Laboratory site. Driven by the need for a sound scientific basis to assess and manage groundwater resources, the Laboratory is conducting analyses of groundwater resources based on data collected from 23 deep monitoring/characterization wells in the regional aquifer across the Pajarito Plateau and from numerous existing wells located throughout the region.

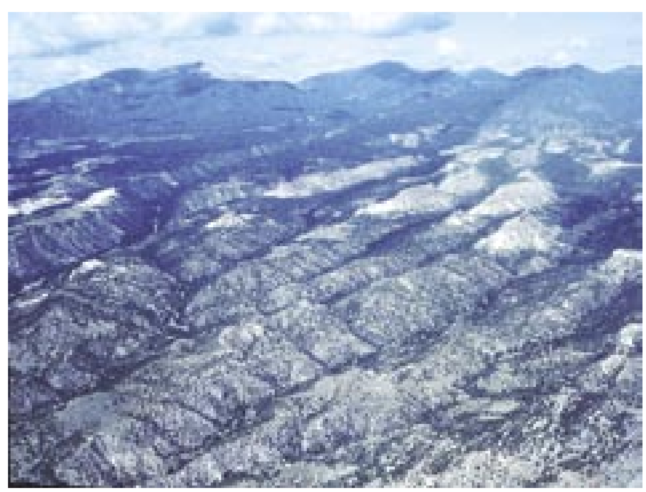
Los Alamos Innovation: Creating a Basin-Wide Model for Testing, Analysis, and Prediction

With its capabilities in geoscience, hydrology, modeling, risk management, and computational analysis, Los Alamos is well suited to create a 3-D model of the geologic framework and a sophisticated hydrologic model of the aquifer. The hydrologic model encompasses the entire Española Basin and includes

- Major stratigraphic units,
- Major water-cycle components,
- Topographic control on the watershed boundaries,
- Flow and transport components for both the vadose zone and the regional aquifer, and
- Accurate predictions of the combined impact of groundwater withdrawals from water users in the basin.

To maintain consistency in scientific approaches and provide technical recommendations to principal investigators and project managers, a Laboratory-wide Groundwater Integration Team (GIT) has been organized to serve as a technical peer review board and a collaborative configuration control board for technical information.

The Laboratory is located on the Pajarito Plateau which is made up of finger-like mesas separated by incised canyons.



The Impact: Insight on Groundwater Resources

Los Alamos's characterizations of the Pajarito Plateau are enhancing our understanding of northern New Mexico's regional groundwater resources and hydrogeology. It is also helping Laboratory site environmental programs comply with regulations by estimating the fate of legacy contaminants in groundwater.

Los Alamos's models have also allowed for sighting sentry wells near water supply wells at risk of future contamination while providing insight into impacts of pumping municipal supply wells on the Pajarito Plateau and other existing wells in the basin. The modeling has also served surrounding communities and pueblos by illustrating and communicating water resource information and providing tools for making water resource management decisions.

Understanding Uncertainty in Water Resource Prediction

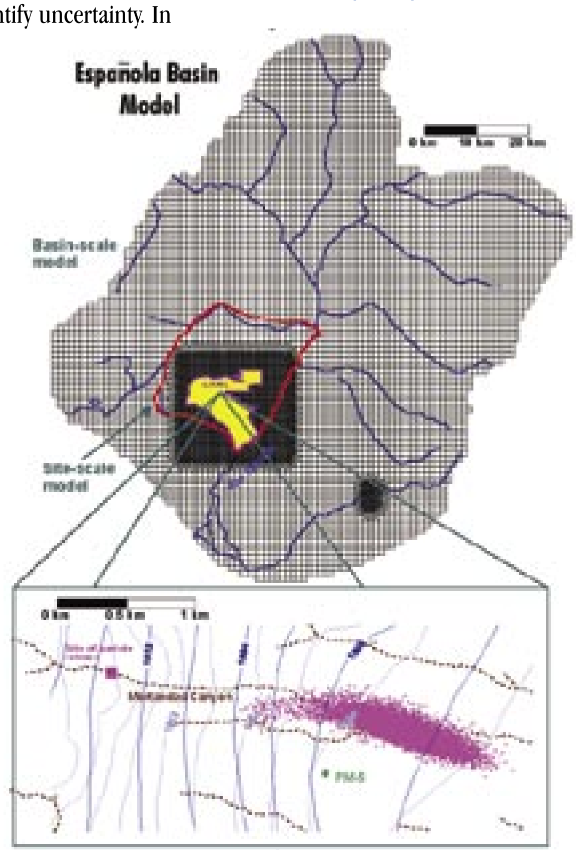
The Challenge: Estimating Predictive Uncertainty in Water Resources Modeling

Models are widely used to understand and analyze the behavior of physical systems and are particularly crucial to water resources research. Significant improvements in groundwater modeling capabilities have allowed for predictions based on more accurate simulations of complex processes. Relatively little attention, however, has been paid to a key aspect of model application: estimating predictive uncertainty. The uncertainty in predictions can be significant when models depend on uncertain knowledge about the modeled system and its governing processes. Los Alamos is developing new methodologies to provide not only water resource predictions, but also robust estimates of prediction uncertainty. Since models and their predictions are used widely in any decision-making process, careful analysis of model predictions and their uncertainty is of great importance.

Los Alamos Innovation: Developing Inverse Models to Quantify Uncertainty

Los Alamos has developed complex forward models which predict system behavior given a set of model parameters, and complex inverse models which estimate the model parameters (recharge rates, aquifer permeability) given a set of system measurements (i.e., calibration data, such as water levels in wells and streamflow measurements). To quantify the sensitivity and uncertainty in the calibrated inverse model is computationally intensive. Therefore, these models require robust information systems and complex coding, both of which are available and were developed at Los Alamos. The Laboratory uses two analytical approaches to the inverse model to quantify uncertainty. In constrained nonlinear optimization, plausible solutions are sought that maximize and minimize given model predictions, allowing prediction uncertainty to be quantified. In inverse-inverse analysis, which Los Alamos is developing, the set of calibration data required to produce a given model prediction with a specified degree of uncertainty

- Overcomes limitations associated with non-linearity of the forward model and non-normality and non linear correlation of the errors;
- Reveals the sensitivity of model parameters and predictions to the calibration data;
- Illuminates the impact of measurement error in calibration data on the inverse estimates and predictions; and
- Extends to quantify the sensitivity of inverse model estimates relevant to general system knowledge, including the uncertainty caused by measurement or conceptual errors.



Plan view of model domains and grids. Inset shows a portion of the model where predictive uncertainty analysis of potential contaminant transport is performed.

The Impact: Improving Diverse Modeling Efforts with Los Alamos Methodologies

The methodologies developed under this project estimate prediction uncertainties and identify key areas where improvements in our understanding of studied systems would decrease the uncertainty in the model predictions. The approaches developed under this project apply to a wide range of problems, including the Los Alamos Española Basin study, which deals with the aquifer in the Los Alamos region. Most of the national laboratories undertake projects that focus on developing models and making important predictions and conclusions using these models. As a result, the Los Alamos project is essential for the laboratories as they work toward the future of the nation.

Plant Cover Effects on Water Resources

The Challenge: Addressing Climate Change and Energy Issues

The United States Global Change Research Program (USGCRP) has identified the water and carbon cycles as national research priorities for the next 10 years. Within the water cycle, hydrological and ecological processes of dry land ecosystems are tightly interrelated. Many important relationships center on the effects that plant cover has on the water budget; for instance, changes in plant cover can trigger high rates of soil erosion. The Laboratory's involvement stems from addressing local environmental restoration needs, obtaining competitive grants within Los Alamos and the Department of Energy, and developing a terrestrial carbon sequestration program with the National Energy Technology Laboratory.

Los Alamos's activities include

- Field experiments;
- Long-term monitoring of soil moisture, runoff, plant water stress, and ground cover;
- Simulation modeling;
- Analysis of historical aerial imagery; and
- Theory development.

The goal is to better quantify the interrelationships between vegetation pattern and dynamics with hydrological pattern and dynamics.

Los Alamos Innovation: Plant Cover and Water Budget Relations

To achieve this goal, the Laboratory is applying its strengths in the area of plant cover and water budget relations. In conjunction with its capabilities in high-resolution hydrological modeling, the Laboratory offers

- The longest-term soil moisture data set for a semi-arid woodland;
- The best-documented example of a drought-induced ecotone shift;
- An experimental drought plot;
- The most intensely studied piñon-juniper woodland site; and
- Biophysical scaling relationships.

The Impact: Effective Land and Water Management Under Changing Conditions

The Laboratory can use a variety of data to address diverse issues, including

- Contaminant transport;
- Drought impacts management;
- Land use in semiarid environments;
- Global change impacts; and
- Terrestrial carbon management and sequestration.

Mesita del Buey Woodland Research Site at Los Alamos National Laboratory where a data set, spanning more than 15 years, has been compiled on soil water and associated plant relationships.

Improved Water Conservation with Waste Materials

The Challenge: Using Plants to Reclaim Mine Sites and Manage Atmospheric Carbon

The United States Global Change Research Program has identified the carbon and water cycles as national research priorities, and the two cycles are strongly intertwined. Energy production and use, which is largely responsible for current imbalances in the carbon cycle, uses as much water as agriculture, and most of the costs of water treatment and distribution can be attributed to energy use. One part of achieving a sustainable water and energy future is the development of plants with optimal water efficiency. Because plants capture CO_2, a greenhouse gas, they play an important role in mitigating climate change. Water-efficient plants can serve double duty at the beginning and end of the energy cycle by revitalizing reclaimed mine sites and by capturing CO_2 produced by energy generation and use. A multidisciplinary team of Los Alamos researchers collaborated with site reclamation experts from the State of New Mexico Abandoned Mine Bureau and examined the potential of using coal mine site spoil and other waste materials to achieve improved vegetative growth and productivity.

Los Alamos Innovation: Using Mine Waste Material as a Beneficial Soil Amendment

As Los Alamos researchers have pursued reclaiming western mine sites for vegetative growth, they have found that waste from these sites is high in nitrogen but does not hold water well, making it a poor vegetation producer. Native western soil, on the other hand, contains clay and holds water well, but is low in nitrogen, making it a poor vegetation supporter. With their expertise in isotopic signatures and using a multidisciplinary approach, Los Alamos researchers have been able to distinguish the carbon from coal from carbon derived from plants at mine sites. Los Alamos has also addressed the potential of using western mine site material to stabilize native alkaline soil to establish vegetative cover while combining native soil and mine site spoil to test its ability to support plant growth in water-limited regions.

Coal mine “gob” piles at Madrid, NM.

The Impact: Plant Growth in Water-Limited Systems

Results of this study reveal that native plants grown in combinations of coal mine spoil and native soil are outperforming those grown solely in native soil or solely in mine spoil. Further work in this area will lead to

- Reduced costs for mine site reclamation;
- More efficient water use when stabilizing reclaimed mine sites;
- Effective management of water in arid land where nitrogen is sparse;
- Beneficial use of waste materials; and
- Reduction in atmospheric carbon through plant capture and storage.

Jemez y Sangre Water Planning Council

The Challenge: Regional Water Planning

In 1987, the New Mexico legislature enacted a statute enabling regions in the state to plan their water future, and in 1998 the Jemez y Sangre Water Planning area was established. Water planning was initiated at the regional level so that unique characteristics of each region would be protected. As a major water user in the planning region, Los Alamos National Laboratory actively participated in developing the Jemez y Sangre Regional Water Plan. The Interstate Stream Commission accepted the plan in April 2003. The Council is in the initial phase of implementing the plan.

Los Alamos Innovation: Providing Leadership in Water Resource Issues

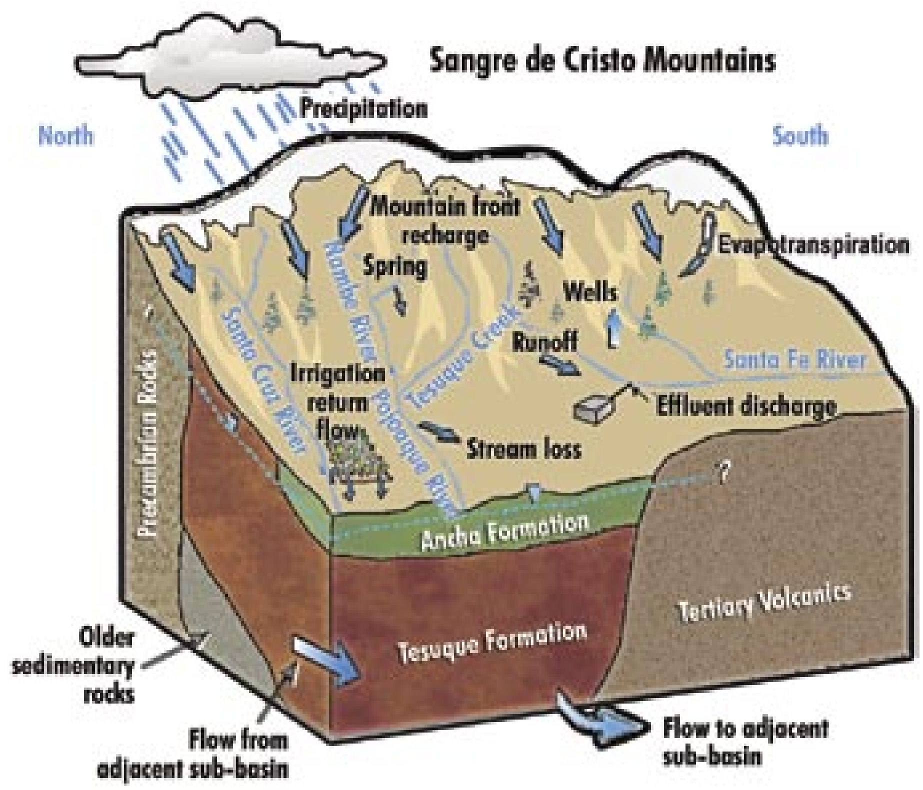
The Laboratory chairs the Water Planning Council and also participates in the subcommittees that focus on understanding sustainable ground and surface water use, provide education, and assess implementation performance.

The Laboratory also chairs the executive committee. Los Alamos's participation in the Jemez y Sangre Council provides additional insight into New Mexico's water resource issues and provides opportunities to apply Laboratory capabilities to resolve those issues.

The Impact: Securing Water Supplies for the Next 60 Years

The regional water planning efforts of the Jemez y Sangre Council resulted in the development of an inventory of the quantity and quality of water resources in the Jemez y Sangre region. Projected water resource demands, responding to a range of conditions, were calculated as a result of these efforts.

The council also recommended alternatives to close the projected gap between supply and demand through 2060 by managing and conserving the region's available water supplies under existing rights, water supplies, interstate agreements, and court decrees. The sum of these efforts will help secure a sustainable water supply for future generations by implementing recommendations in the water plan.



Conceptual model of the Jemez y Sangre Water Planning region.

New Mexico Governor's Blue Ribbon Water Task Force

The Challenge: Long-Range Planning for New Mexico's Water Resources

New Mexico is an arid state with a limited amount of available water. Long-range planning and policy making is critical to ensure an adequate water supply for New Mexicans for generations to come. To meet New Mexico's planning needs, the Blue Ribbon Water Task Force was established.

Los Alamos Innovation: Science-Based Advice for State Water Planning

As requested by Governor Bill Richardson, Los Alamos National Laboratory provides two members to this task force. The purpose of the task force is to investigate and engage in discussions regarding current water policies and laws implemented within New Mexico.

The council has also been tasked with advising the State Engineer, Interstate Stream Commission, and any other relevant state agencies, regarding water policy and laws in relation to the implementation of the State Water Plan. It provides the Governor, State Engineer, and Interstate Stream Engineer with its recommendations every November.

The Impact: Science, Law, and Public Policy Working in Concert

Water management goes beyond understanding physical, natural systems alone. The Blue Ribbon Task Force will help untangle the web of legal, economic, and policy issues that are intertwined with scientific and technological solutions.

The Blue Ribbon Water Task Force will provide water policy and law recommendations annually to New Mexico's Governor.

DOE Water Cycle Pilot Study

The Challenge: Understanding Regional and Global Hydrological Cycles

Los Alamos National Laboratory co-chaired the committee that produced the Department of Energy's (DOE) Water Cycle Initiative Research Strategy, which defined the agency's role in the U.S. Global Change Research Program's Water Cycle Study. The successful collaboration between Los Alamos and the larger team led to a pilot study funded by the DOE. The Water Cycle Pilot Study is focused on the Whitewater River Basin in Kansas, which is part of the DOE ARM (Atmospheric Radiation Measurement) Southern Great Plains site. It began with the goal of improving model parameters and our physical understanding of the water cycle through process studies, new observational methods, and field sites that provide continuous long-term data streams.

Another goal is to couple models in a high-performance computing environment, link domain models across processes (physical, chemical, geological, and biological) and scales (global, regional, local) and to provide a modeling and testing environment for DOE and the U.S. Global Change Research Program's research efforts.

Above: View of the landscape in the Whitewater River Basin, Kansas.

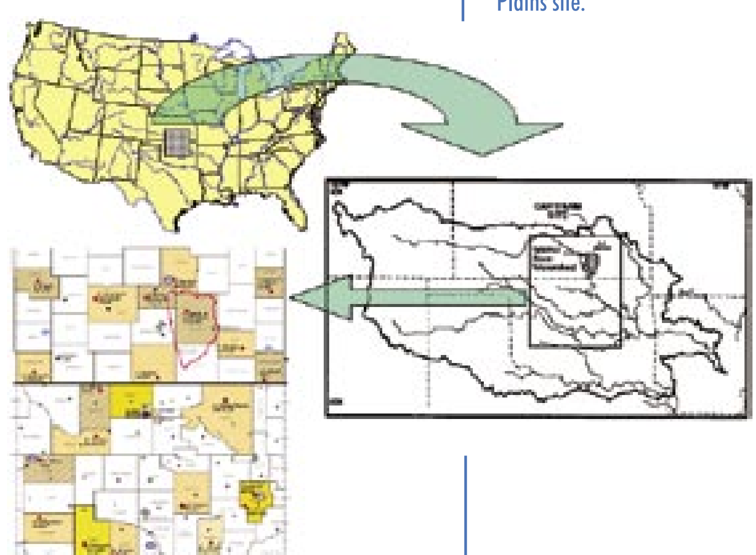
Los Alamos Innovation: Coupling Complex Models

The pilot study was built upon the complementary abilities of the larger team. Los Alamos National Laboratory contributed its high-performance computing and existing capabilities in coupling regional atmospheric and hydrologic models.

Below: A map of the Whitewater River Basin within the DOE/ARM Southern Great Plains site.

The Impact: Predicting the Future of Water Resources

Over the course of the pilot study, researchers will collect and analyze data to assess and predict the effects of climate variability and land use change on water resources. When the study is completed, it will have created coupled models in a high-performance computing environment and demonstrated the capability of integrated teams to address complex problems.



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Los Alamos Hydrogeologic Workplan

The Challenge: Characterizing Los Alamos's Hydrogeological Setting

In response to a request from the New Mexico Environment Department, Los Alamos National Laboratory developed a hydrogeologic workplan that details activities to be performed over a 7-year schedule for a site-wide hydrogeologic characterization. Implementing the workplan would provide sufficient information to adequately design and install additions to the groundwater monitoring network for the site. Los Alamos based the hydrogeologic workplan on the application of the Environmental Protection Agency Data Quality Objective (DQO) process to optimize the data collection design. The workplan depends on an iterative approach—collecting data from a specific borehole and well that will be analyzed and interpreted for sound decision-making on future data collection activities, thereby allowing for project economies and selection of appropriate DQO's.

Los Alamos Innovation: Producing Sophisticated Models to Understand Site Hydrogeology

For each well, the Laboratory develops discrete sampling and analysis plans that detail the DQO's and well design. The completed wells are typically constructed with multiple screens, where instrumentation is used to allow discrete sampling and pressure measurements to be made at different depths. During borehole construction of the 23 regional aquifer wells, at depths near 2,000 feet, the Laboratory has collected

- Geologic samples (cuttings and core) for laboratory analysis;
- A complete suite of geophysical and video logs in the borehole; and
- Water samples for contaminant screening.

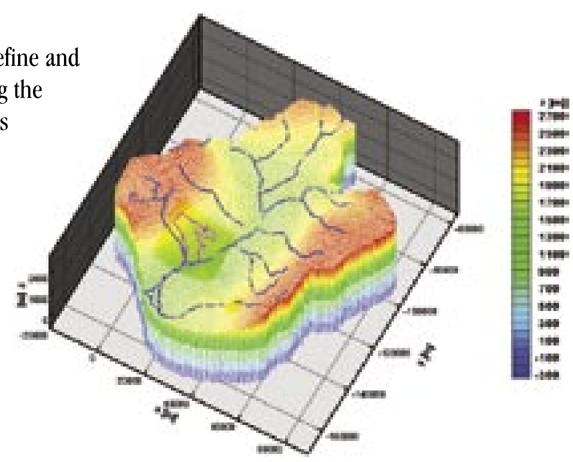
Each well is sampled 4 times during an 18-month period. The high-performance computing and modeling capabilities at Los Alamos are used to produce sophisticated models of the vadose zone and saturated zone. As a result, the Laboratory has derived a comprehensive understanding of the site's hydrogeologic setting.

The Impact: Advanced Techniques to Solve Groundwater Resource Problems

After 6 years of implementing the Hydrogeologic Workplan, Los Alamos has been able to refine and validate the conceptual model of the Pajarito Plateau hydrogeologic setting while increasing the efficiency and cost effectiveness of the drilling process. In addition, data collection activities through the iterative DQO process have been enhanced. Another result has been the development of useful tools for performing risk assessments and protecting groundwater resources. The site-wide characterization has been completed ahead of schedule.

Collaborating with regional government agencies and interested parties, the Laboratory is contributing its expertise and knowledge to solve problems on a regional basis in the Española Basin. Additionally, the experience gained by the Laboratory in conducting such a large-scale site investigation is directly transferable to other sites and locations where it can be used to develop solutions for related ground-water resource management questions and problems.

Española Basin model 3-D grid with elevations and the Laboratory's boundary highlighted.



Future Directions

Water Management

The Earth's abundance of water belies its small availability. While two-thirds of the planet is covered in water, only 2.5 percent is fresh, and only 1 percent is readily accessible. Pollution further reduces this number, and population increases mean more demand. With national security and global stability in mind, Los Alamos National Laboratory has identified the critical issues and the science and technology to address water problems in the United States and the World.

Los Alamos National Laboratory Water Program Strategic Goals

Water for Energy
The energy industry is second only to agriculture in water use, and population growth strains water resources through both direct use and increased energy demand. Leading the way in identifying key challenges to energy and water supplies, Los Alamos engages industry and water regulators across the country, performing in-depth analyses to identify real-world problems and solutions, such as

- Decision support tools for water and energy policymakers,
- Technology to reduce water use,
- Access to untapped resources, and
- Water quality assurance.

Through industry and government partnerships, solutions will move into the marketplace and planning community.

Water Security
Health and economic development depend heavily on the quantity and quality of water resources. Los Alamos is applying its expertise to homeland defense to address new threats in a changing world. Los Alamos is improving its ability to predict, prevent, and respond to attacks on the nation's water supplies.

Regional Water Cycle
Los Alamos partners with universities, private industry, and government agencies to understand potential changes to water resources. The Laboratory is working with the atmospheric sciences community to develop models to simulate the global ocean and climate system. A detailed understanding of the climate response will allow regional simulations to assess local effects of climate variability and land use change. Integrated regional models, designed at Los Alamos, represent the atmosphere, landscape, and subsurface with accuracy, so locations and times for effective implementation of mitigating actions can be identified. Los Alamos is creating techniques to measure evaporation and water quality across basins, enhancing predictive capabilities, and providing a better account of regional water. The results of this initiative will support future water use plans and resource managers in their tasks.

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